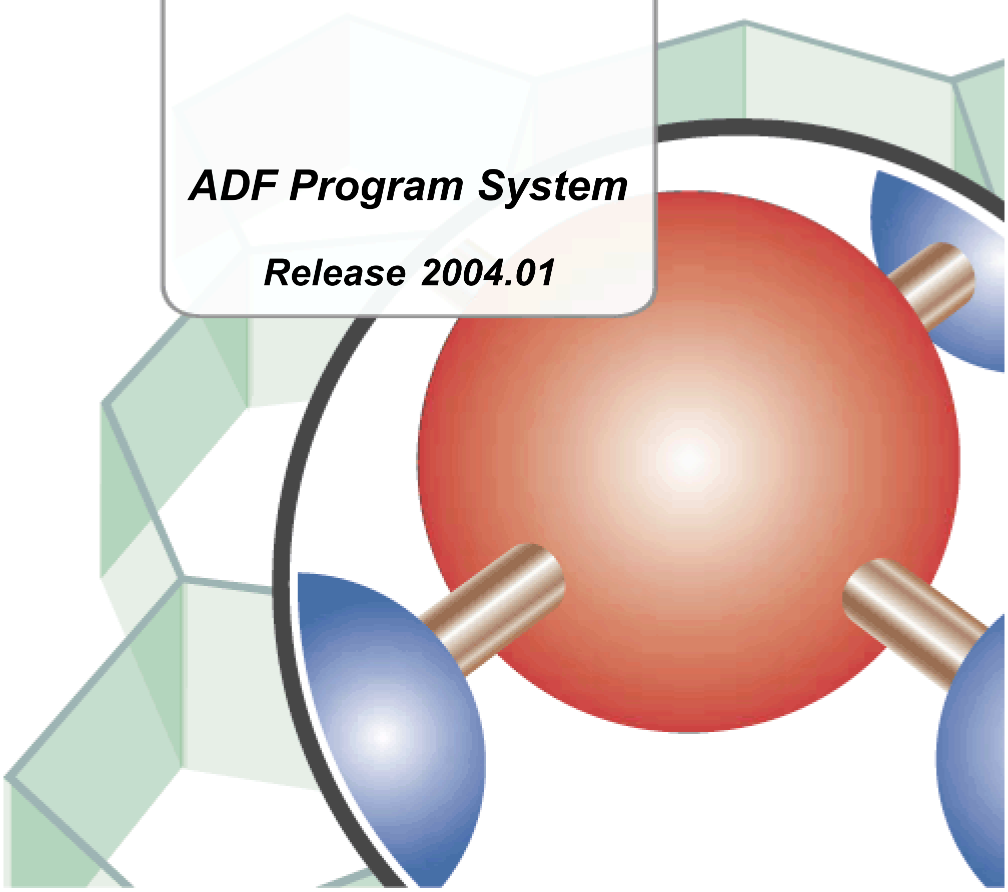
Scientific Computing & Modelling

ADF GUI Tutorial



ADF Program System

Release 2004.01

Table of Contents

Introduction

This document will provide a basic hands-on tutorial of the ADF GUI. Its purpose is to give a quick tour of the main features of the ADF GUI.

It consists of three main sections: an ADFinput tutorial, and ADFview tutorial and an ADFspectra tutorial. If you are new to the ADF GUI we advise you to study these tutorials in the order presented.

We estimate that you will need about half an hour for each part of the tutorial, for reading and performing the hands-on activities. Thus for the entire tutorial you will need about one and a half hour.

Additional information may be found in the ADF GUI Reference manual, especially about ADFinput and ADFview.

ADF GUI modules

ADF GUI is the Graphical User Interface for the ADF package. It consists of several modules:

`ADFinput`

> A utility program, which enables ADF users to easily create ADF jobs. You can use ADFinput to define your molecule (geometry), pre-optimize it, and to set details of your ADF job using an easy-to-use graphical user interface. ADFinput will generate the complete job script for you. This script takes care of running ADF and property programs as required. You can also use ADFinput to run these script files on your localhost in the background.

`ADFview`

> A simple program that displays 3-D (volume) data, such as electron densities, orbitals, electrostatic potentials.

`ADFmovie`

> This program follows geometry steps as performed by ADF during geometry optimizations, IRC calculations, etc. Actually, it will display just any series of changing geometries, and is also used to display normal modes calculated with a frequency calculation.

`ADFspectra`

> Show the spectra calculated by ADF. Currently it can show IR and excitation spectra, as well as a DOS plot. For some spectra (for example for IR spectra) it can also provide additional information, like a visualization of the normal modes (using ADFmovie). More types of spectra will follow in future versions.

`ADFtail`

> A minor GUI utility that will just show the contents of a text file, updating when the text file grows. It is used to follow the progress of an ADF calculation (similar to the UNIX tail -f command)

`BOB`

> A Basic Output Browser for the output generated by ADF.

All ADF GUI modules have the SCM menu on the left-hand side, on most systems represented by a small SCM logo. Using the SCM menu commands you can easily switch between the different modules of the ADF

GUI.

ADF installation

We will assume that you have installed the ADF package on your machine, and that you are familiar with running ADF jobs.

In this tutorial we assume that you have added $ADFBIN to your PATH. We advise you to do this if you have not already done so. If you wish not to add $ADFBIN to your PATH, you must start the utilities using

```
$ADFBIN/adfinput &
```

instead of just adfinput &.

On all UNIX platforms, including Mac OS X, the ADF GUI programs are XWindow programs. Your environment should have been set up correctly to run such programs. In particular, you need to make sure that your DISPLAY environment variable has been set properly.

You can test this easily by starting a simple X program from your shell:

```
xcalc &
```

Assuming the xcalc program is in your $PATH, a small window should appear with the image of a calculator. If not, please consult your local system administrator for additional help. Typical problems have to do with your DISPLAY variable, and with security issues when trying to connect to the X server.

The ADF GUI is available for all platforms for which ADF 2004.01 is available.

Automatic bug-reports

Please enable the automatic mailing of bug-reports. These reports contain detailed information about the internal state of the GUI module having some problem, but do not contain personal information.

You can enable this by setting the global environment variable SCM_ERROR_MAIL, for example in your login script:

```
SCM_ERROR_MAIL=errors@scm.com
export SCM_ERROR_MAIL
```

This will ensure that the bug report will be sent to the mail address you specify. If you specify your own email address you can see exactly what kind of information is contained in the error report. And of course we would like you to forward that report to errors@scm.com.

Your comments and bug reports are very welcome. Please send them to support@scm.com.

ADFinput tutorial

This tutorial will help you to:

- create a molecule with ADFinput
- make some changes to the molecule
- set up an ADF calculation with ADFinput
- perform the actual ADF calculation
- visualize some results.

Step 1: Start ADFinput

Make a directory for the tutorial

We prefer to run the tutorial in a clean directory. That way the tutorial will not interfere with other projects. Thus:

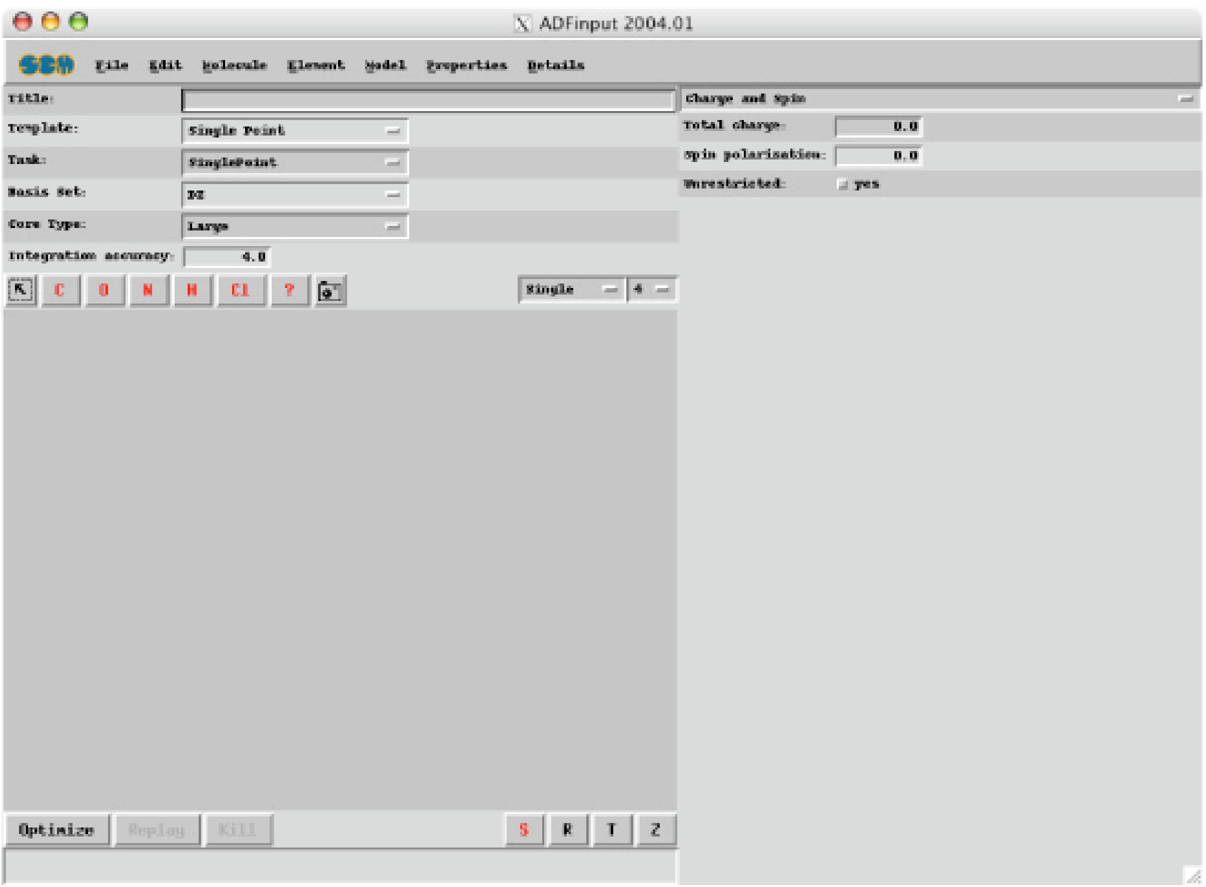
```
mkdir $ADFHOME/tutorial
cd $ADFHOME/tutorial
```

Start ADFinput

Enter the following command:

```
adfinput&
```

This will start the ADFinput program in the background:



The main window consists of the following main parts:

- the menu bar with the menu commands
- the main options (on the top left side)
- the molecule editor with some tools (on the middle left side)

- the status field (on the bottom left, currently empty)
- a set of selected other options (currently 'Charge and Spin')

Step 2: Create your molecule

Create a molecule

Next we are going to create an ethane molecule:

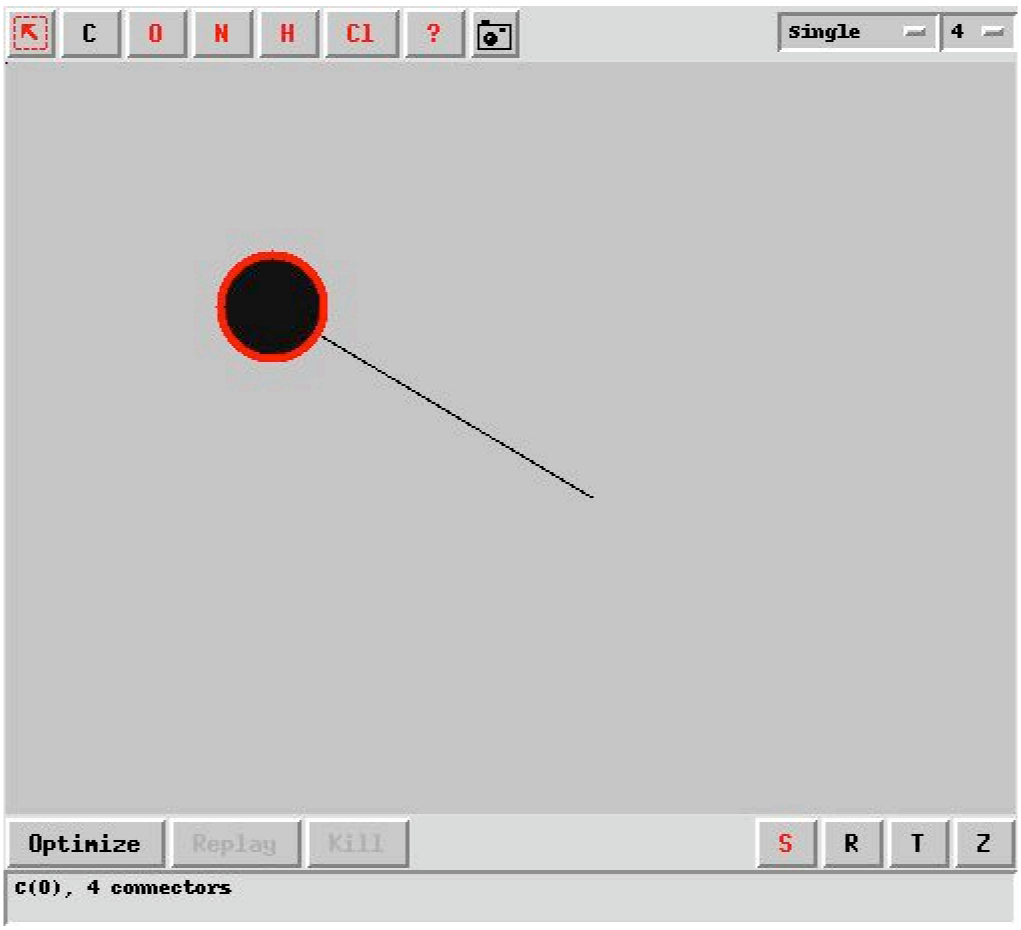
Select the C-tool

```
Select the C-tool by clicking on the 'C' button,
just above the big empty drawing space.
```

The 'C' button is now black to indicate that you are using the C-tool.

Create the first carbon atom

```
Click somewhere in the dark-gray empty space below the buttons.
```



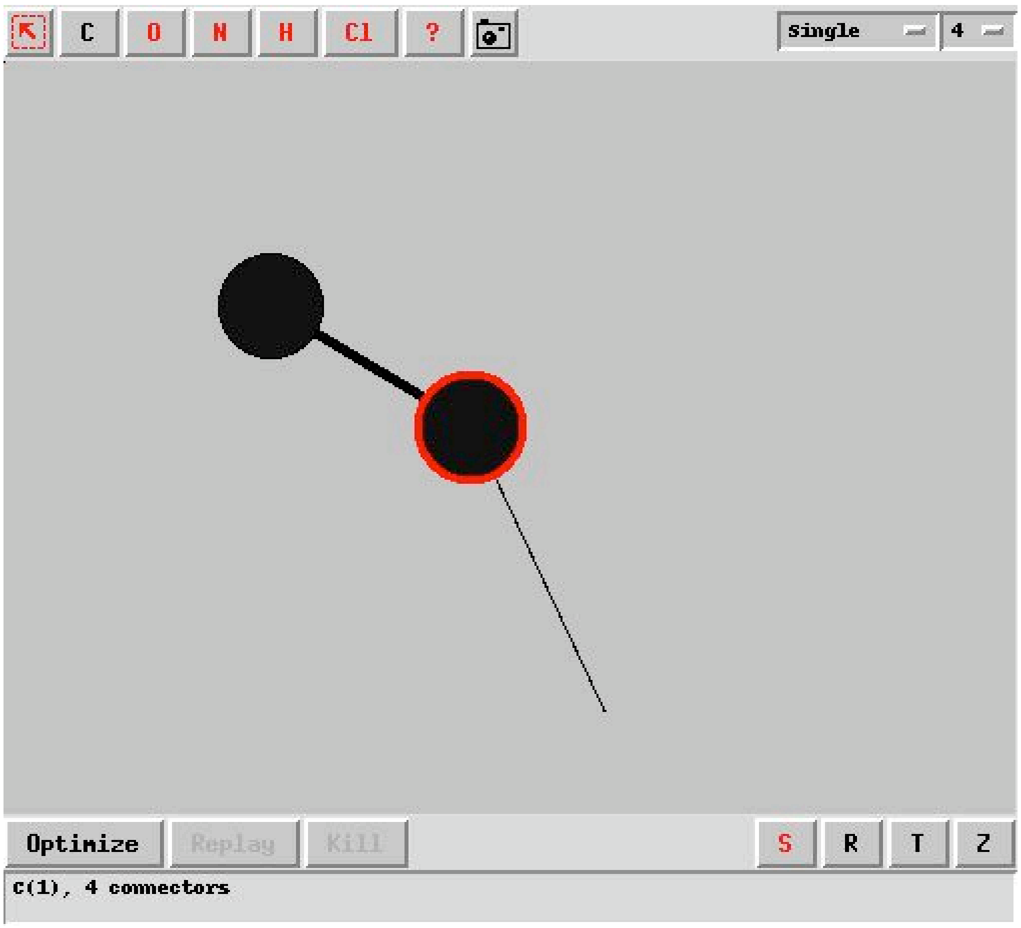
One carbon atom has been created.

Note that:

- If you move the mouse you will see a line from that carbon atom to the current mouse position: this shows you are in 'bonding' mode, and that the bond will be made to the atom just created.
- The 'C' button is black, indicating you are still using the C-tool.
- The red circle around the carbon atom indicates that the carbon atom is the current selection, of one atom only.
- Look at the status field, you can read some information about the current selection: it is a Carbon, number 0, with 4 'connectors'.

Create the second carbon atom

`Click a second time somewhere in the empty space.`



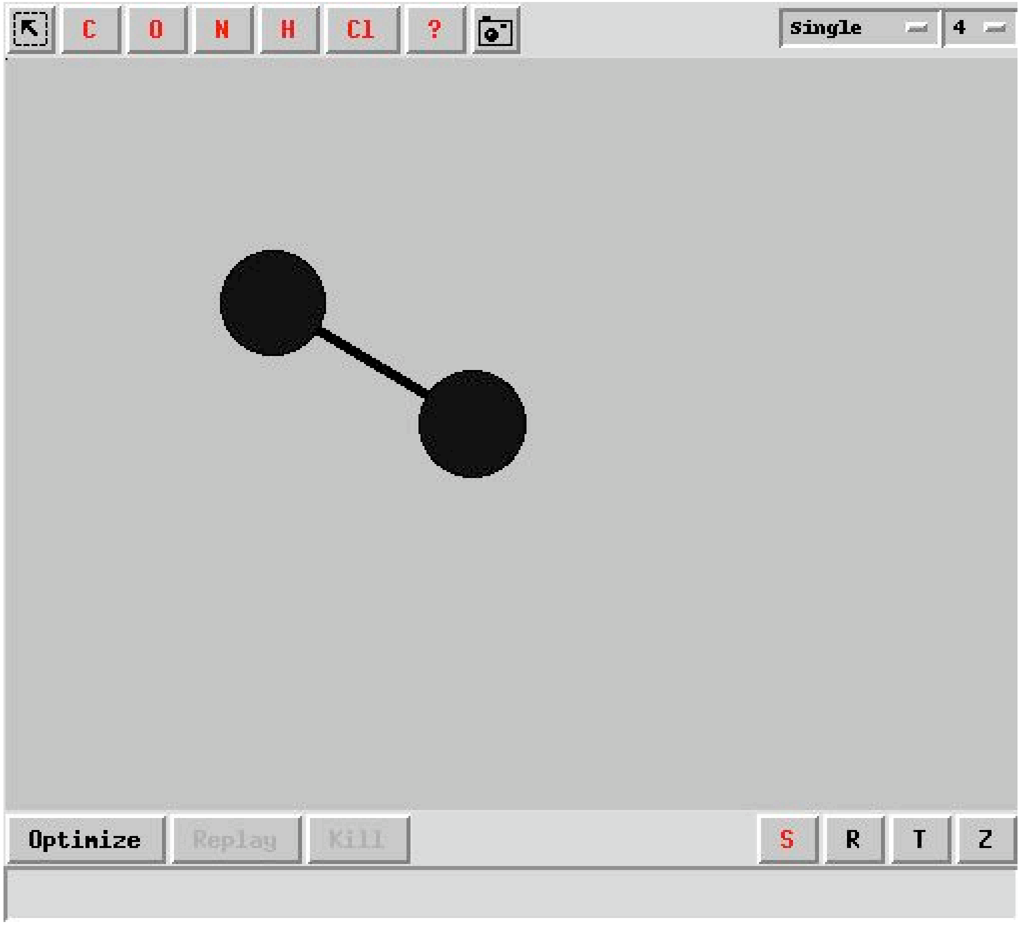
A second carbon atom will be created, bonded to the first atom.

The atom will be created along the 'bonding line', at a distance that corresponds to a normal C-C single bond distance. That is, the bond length is constrained while drawing.

The newly created atom becomes the new selection, and you are still in bonding mode. The next bond will be created to the carbon atom just created. And you are still using the C-tool.

Finish the C-tool mode

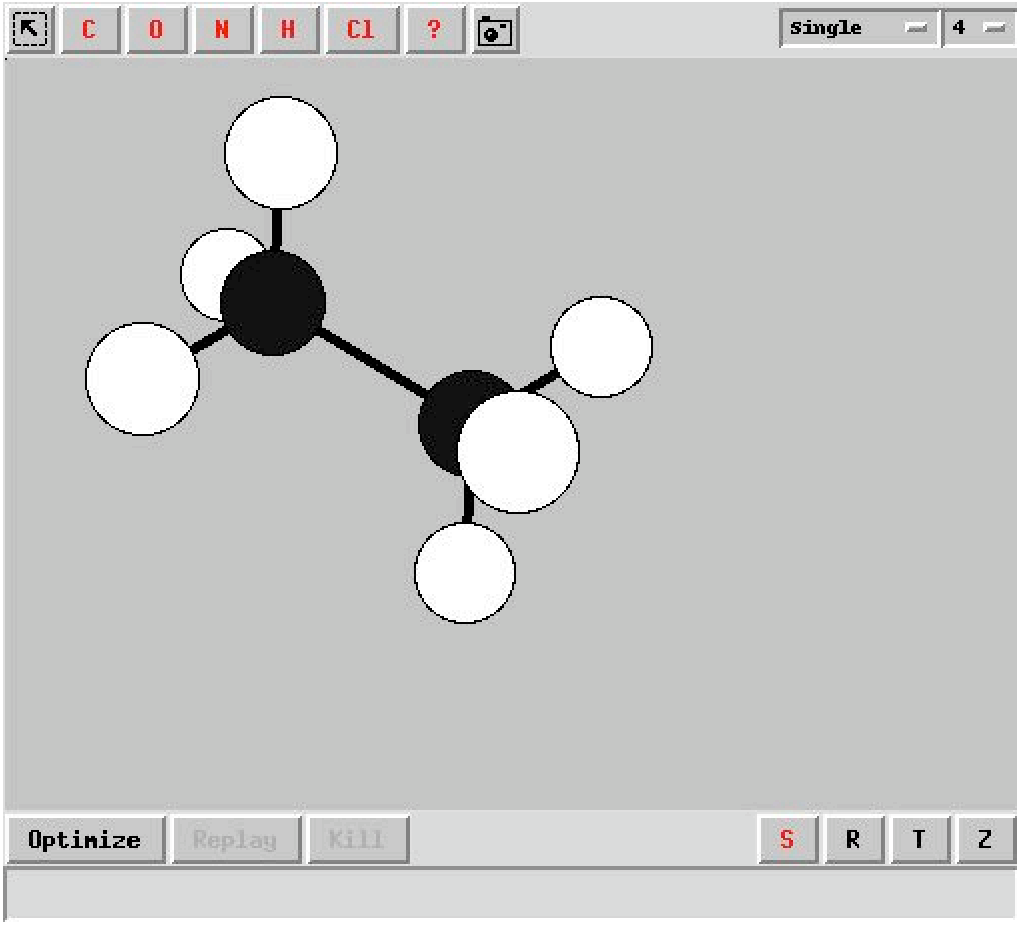
Click once on the currently selected carbon atom.



This ends the C-tool mode, as you can see you are now using the select-tool again.

Add the hydrogens

Select the 'Add Hydrogen' command from the 'Molecule' menu.



You have created an ethane molecule.

Viewing the molecule

The following instructions assume you are using a three-button mouse. If you have a mouse with one or two buttons, check the description of the S, R, T, and Z buttons in the reference manual to learn how to achieve the same effects.

Rotate the molecule

```
Click in the picture and hold down the right mouse button.
```

A red rectangle appears for help with rotation.

```
Move the mouse around
(still pressing the right mouse button!).
```

You will rotate your molecule, and will continue to do so until you:

```
Release the mouse button.
```

Rotating works using a 'virtual trackball': when you move the mouse somewhere in the center, the picture changes as if you were rotating by pushing the top of the ball. If you move the mouse near the edge of the picture (outside the rectangle), the rotation will be around an axis perpendicular to the screen.

Zoom the molecule

```
Press and hold the control key,
click in the picture and hold down the right mouse button.
```

```
Move the mouse to the right
(still pressing the right mouse button and control key!).
```

As the picture of the molecule will show, you are zooming in.

```
Move the mouse to the left
(still pressing the right mouse button and control key!).
```

You are zooming out.

```
Release the mouse button and the control key.
```

Translate the molecule

```
Click in the picture using the middle mouse button,
and hold down the mouse button.
```

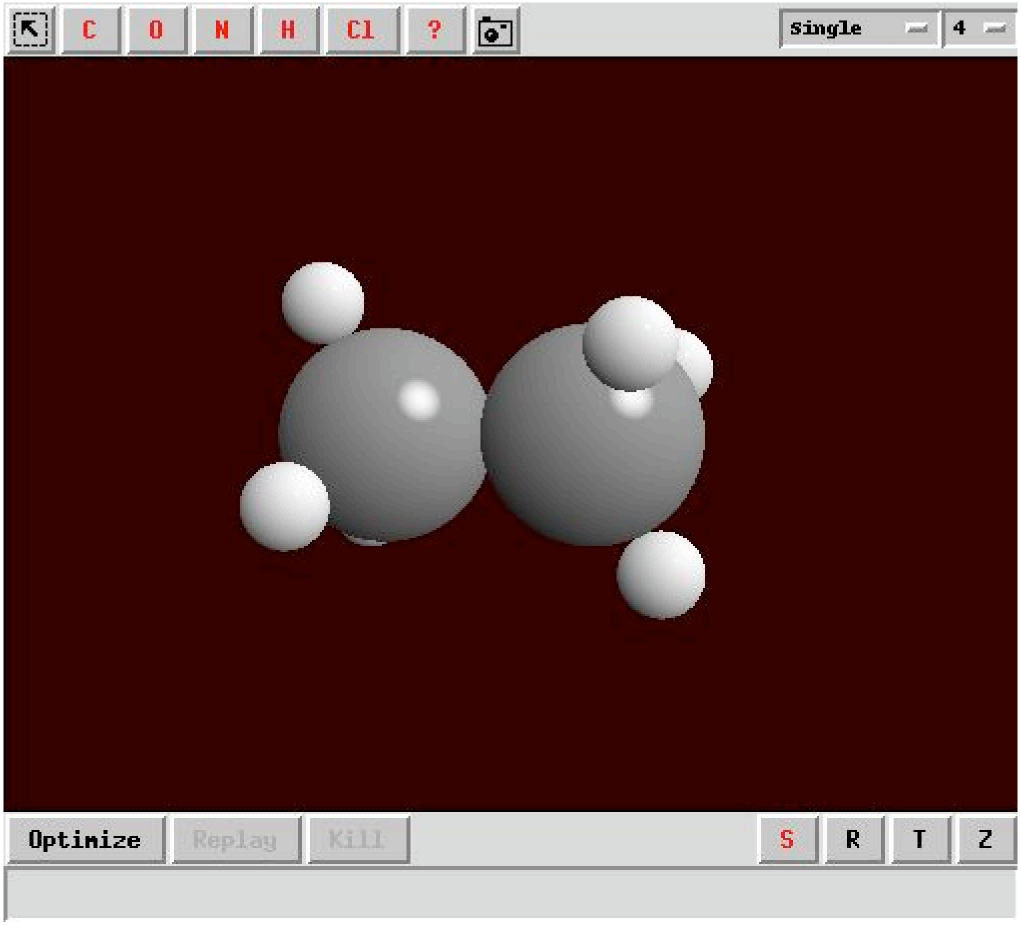
```
Drag the mouse in some direction.
```

The molecule will be translated following the mouse.

High quality image

You can also change the picture of the molecule to a high quality picture. This looks much better, but is also much slower. For that reason you will probably want to edit and move your molecule using the simple (default) display mode.

```
Press the button with the camera icon, next to the button with
the question mark.
```



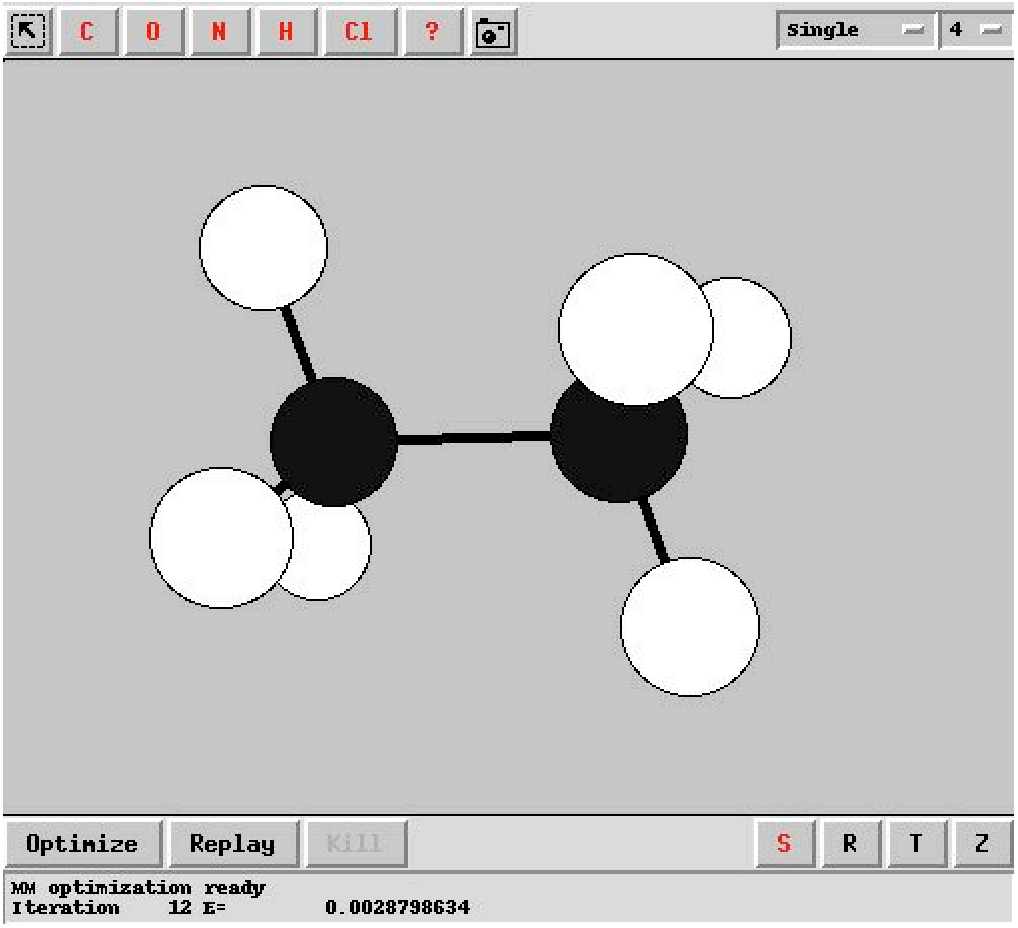
This toggles between the nice and fast picture modes.

`Press the button with the camera icon again, to get back to normal view`

Pre-optimize geometry

```
Click on the Optimize button in the lower
part of the editing window.
```

This will optimize the geometry of the ethane molecule.



The method used for this optimization is a very simple (and not very accurate) optimization using a force field.

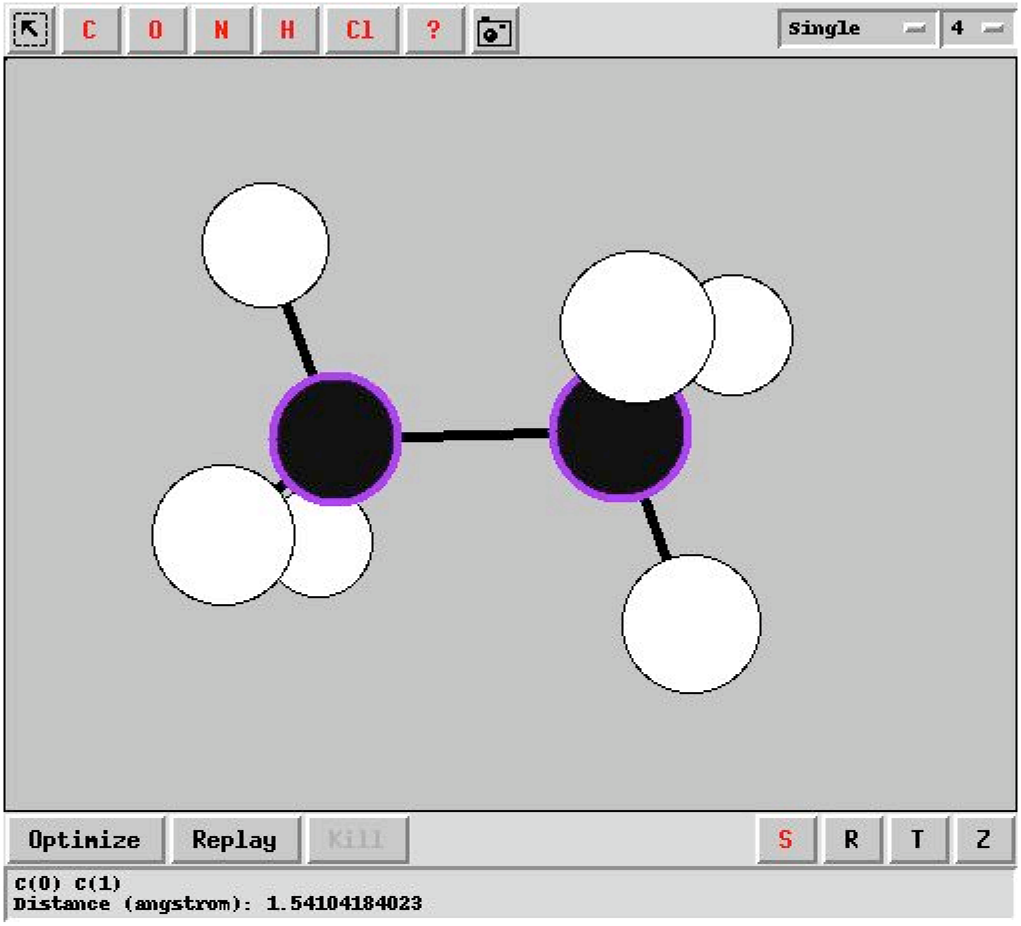
In the status field you can see the results of the optimization. The energy reported is just the force field value and has no physical meaning.

Geometry information

Bond length

Select the two Carbon atoms:

`Hold the shift key, and click once on both carbon atoms.`



In the status field you will find the bond length between the two selected atoms, and the names of the two selected atoms.

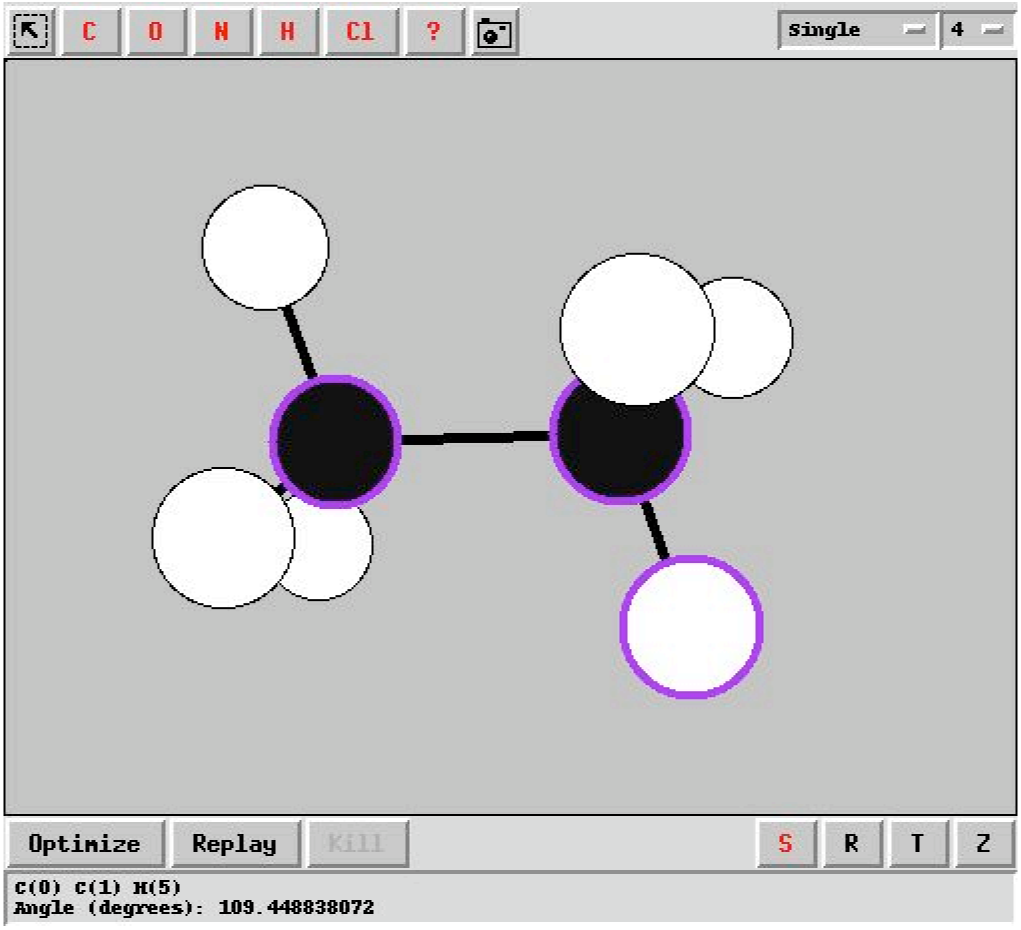
Bond angle

First clear the current selection.

`Click once in empty space.`

Select three atoms:

`Hold the shift key, click once one each carbon, and on a hydrogen.`



In the status field you will read the names of the three selected atoms, and the angle between these atoms. The order in which you select the atoms is important.

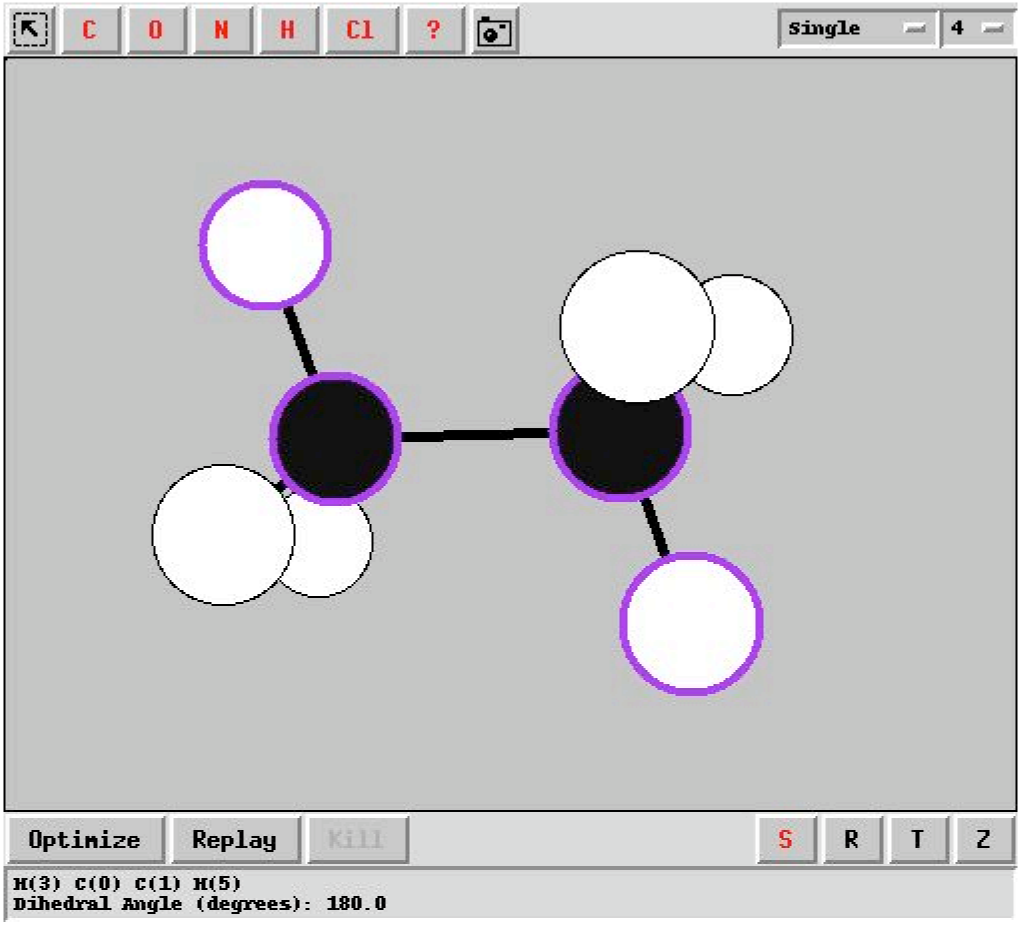
Dihedral angle

First clear the current selection.

```
Click once in empty space.
```

Select four atoms:

```
Hold the shift key:
click once on one hydrogen,
next once on each carbon,
and finally again on a (different) hydrogen.
```



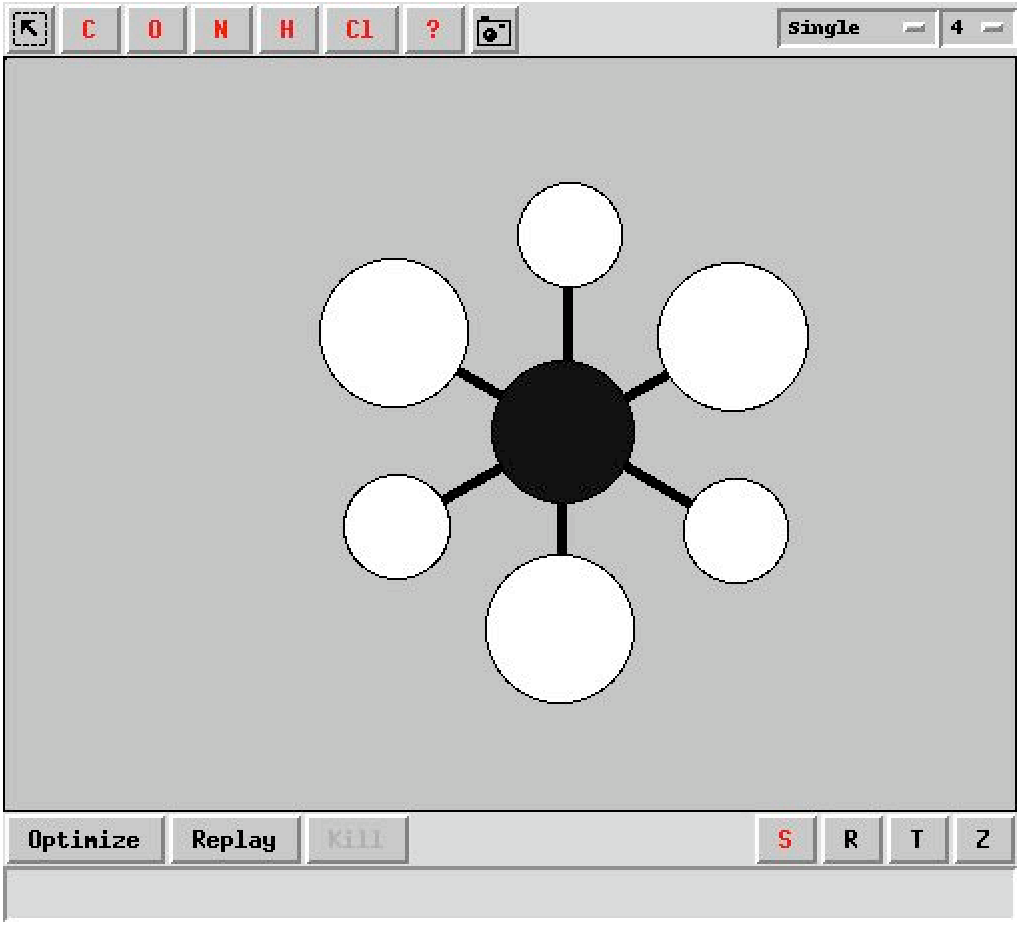
In the status field you will read the names of the four selected atoms, and the dihedral angle between these atoms. The order in which you select the atoms is important.

Changing the molecule

Rotate such that you look along the C-C axis

```
Clear the selection (click in empty space).

Rotate as described before (with right mouse button)
such that the two C atoms are on top of each other.
```

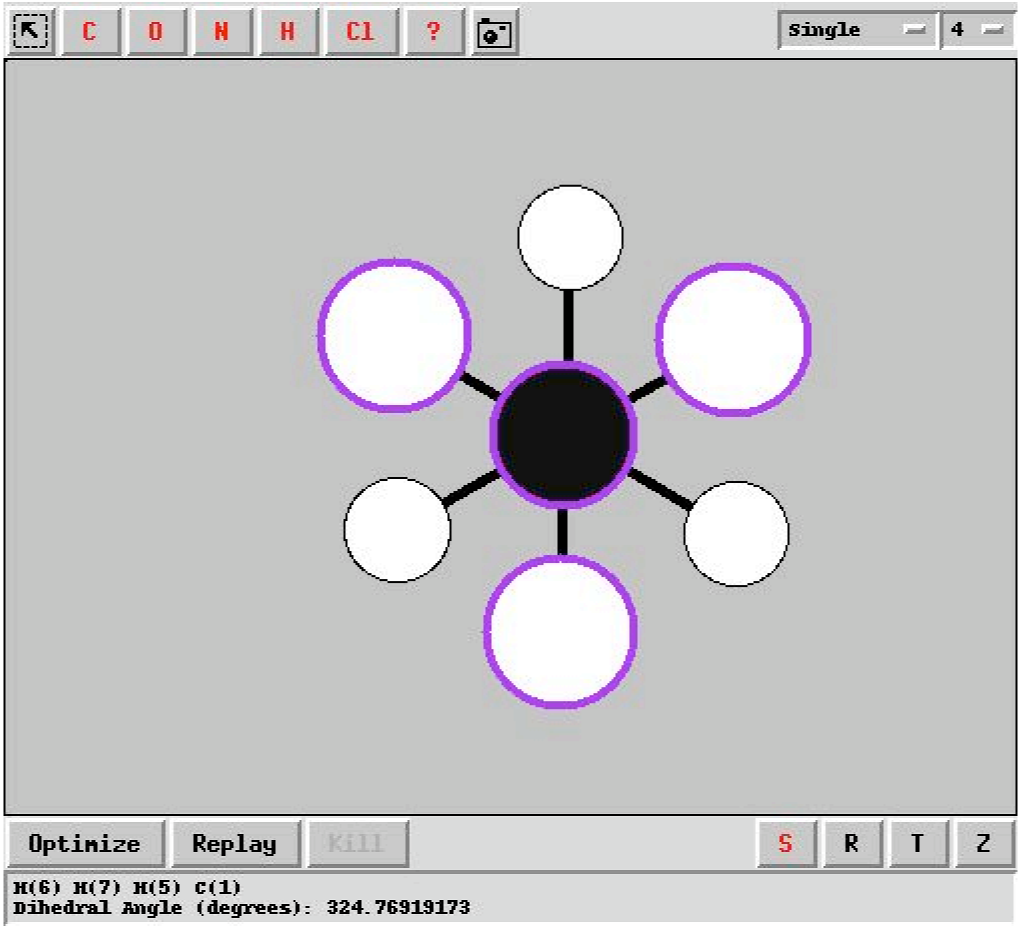


Note that atoms far away are smaller than similar atoms closer to you.

Select the top CH3 group

```
Hold down the shift key, and click once on the top (visible)
C atom, and once on each connected H atom.

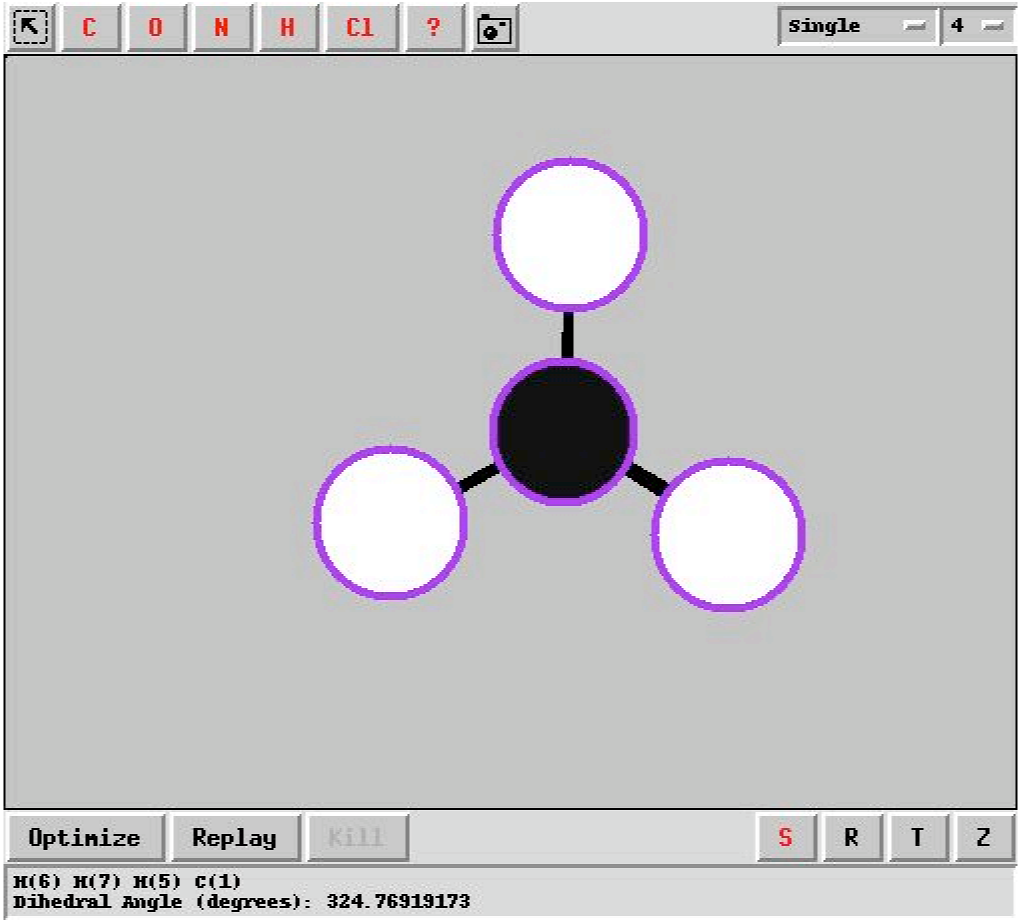
Be careful not to move the mouse while clicking!
```



Rotate the selection

```
Rotate (with right mouse button).
Make sure you move the mouse at the edge of the screen to get a pure rotation.
Rotate until the hydrogen atoms are on top of each other.
```

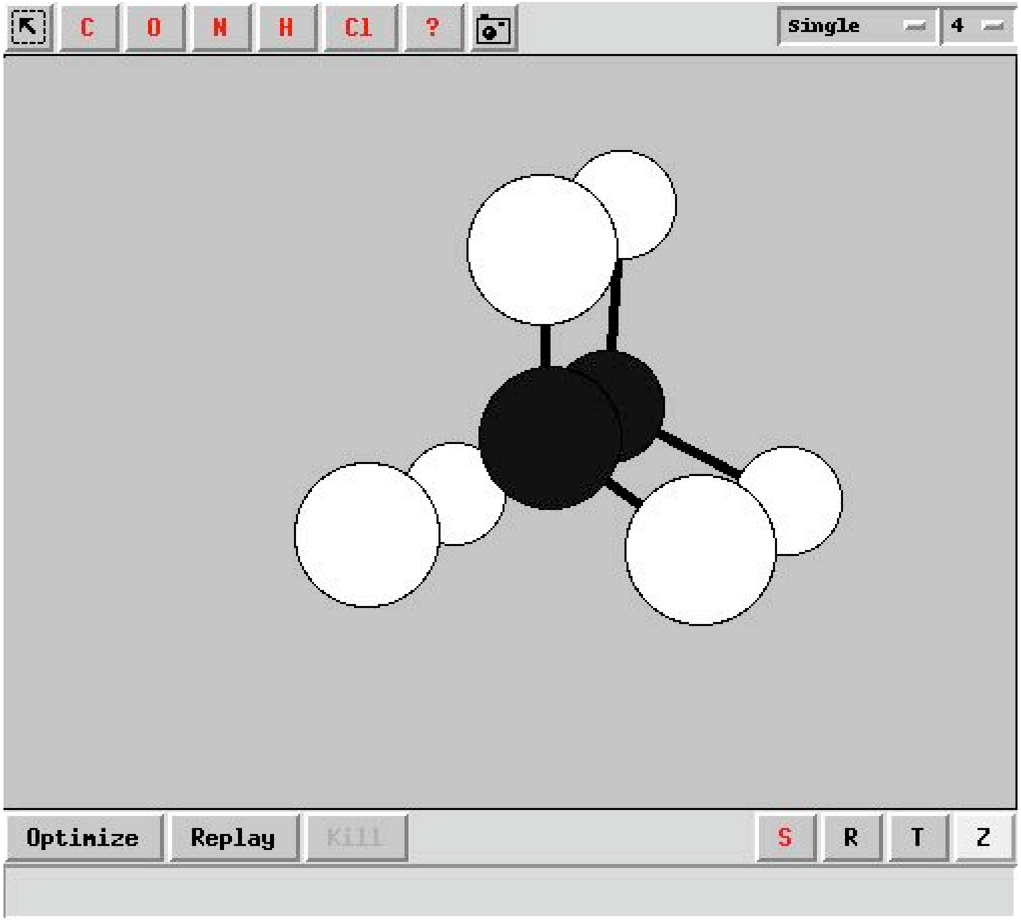
Only the selected atoms will rotate. Your result will look something as the following picture:



Next we rotate the entire molecule a little bit. To do this, you first have to clear the selection (click in empty space):

```
Click in empty space.
```

```
Rotate the molecule slightly.
```

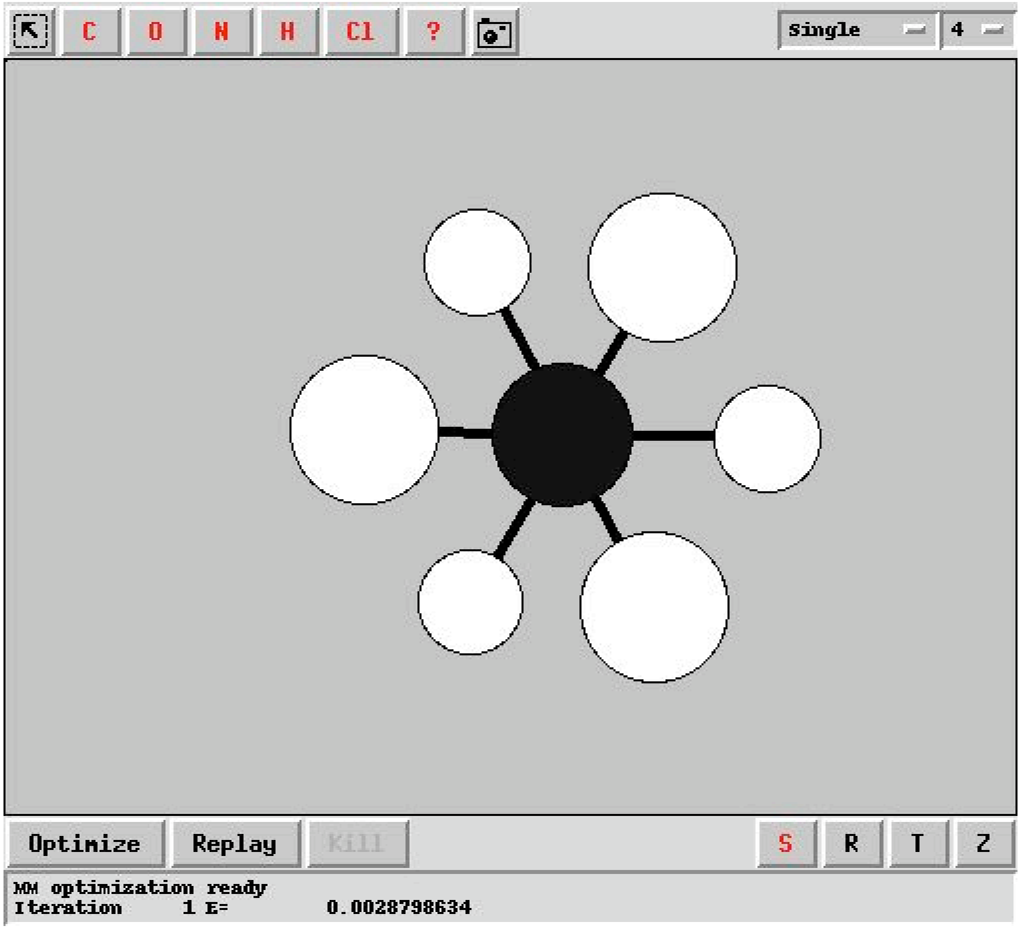


Back to Staggered Geometry

To get back to the staggered geometry, you could do the same trick again. But easier try the following:

```
Click optimize a few times.
```

Typically (not always...) the optimizer will bring back your molecule to the staggered geometry. Unless you managed to bring it into the perfect eclipsed geometry in the previous step, but of course this is not very likely. In that case all forces will balance, and the optimizer will leave the molecule in the perfectly eclipsed geometry.



You need to click optimize more than because the forces in the almost eclipsed geometry are very small, so the optimization algorithm (incorrectly) assumes it is ready too early.

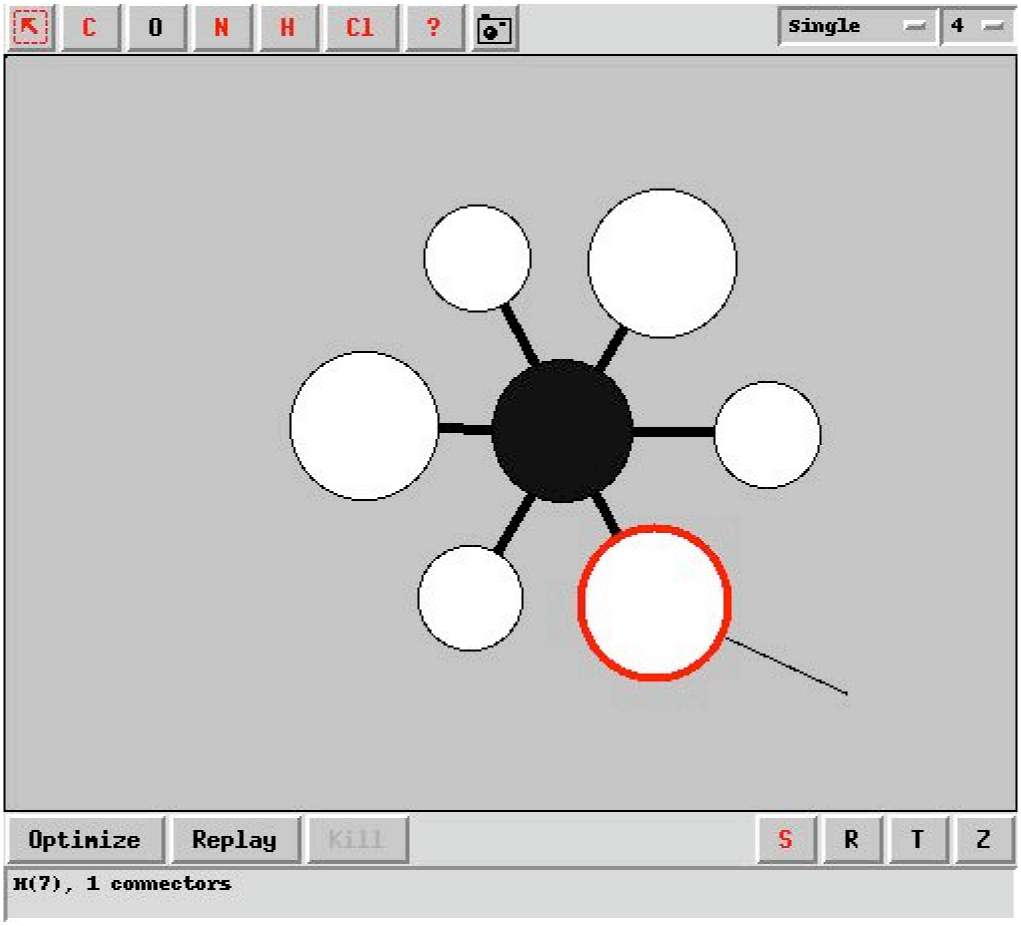
Making ethanol out of ethane

Select the O-tool to create an oxygen atom:

`Click on the 'O' button.`

Change one of the hydrogen atoms into an oxygen atom

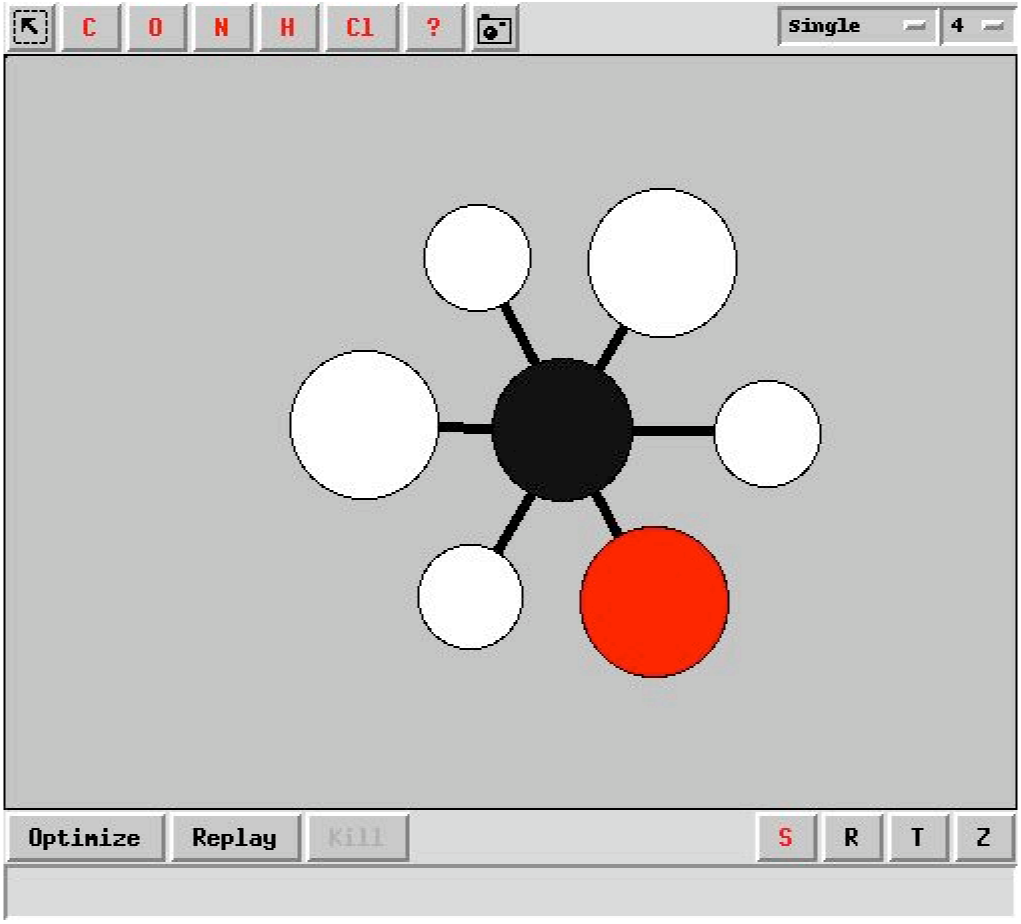
`Click once on a hydrogen atom to select it.`



Note that the hydrogen atom becomes the selected atom, and that you are in bonding mode.

If you would click in empty space, ADFinput would try to create a new oxygen atom bonded to the hydrogen atom. Since a hydrogen atom can only be connected to one other atom only this would NOT succeed.

`Click once more on the same atom to change it into an oxygen atom.`

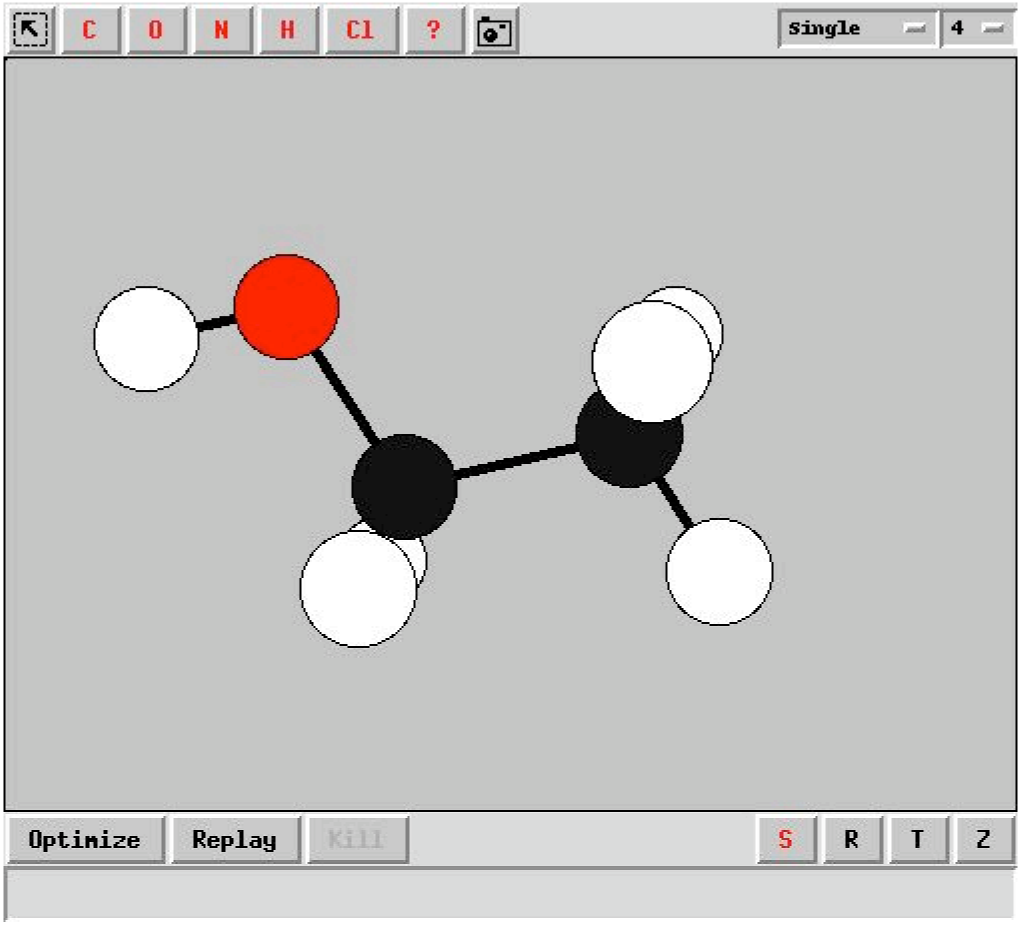


The selected atom will change into an oxygen atom. And since you clicked on the selected atom you will revert to the select tool.

`Choose Add Hydrogen from the Molecule command.`

`Rotate the molecule.`

`Click on 'Optimize' to optimize the geometry.`



Your ethanol is now ready.

Step 3: Select calculation options

Template

You should always start by choosing the proper template.

ADF has many different modes of operation. ADFinput presents the correct settings for some common calculations together as 'templates'.

So to optimize the geometry of the ethanol molecule we just choose the proper template:

`Select the 'Geometry Optimization' template in the 'Template' menu.`

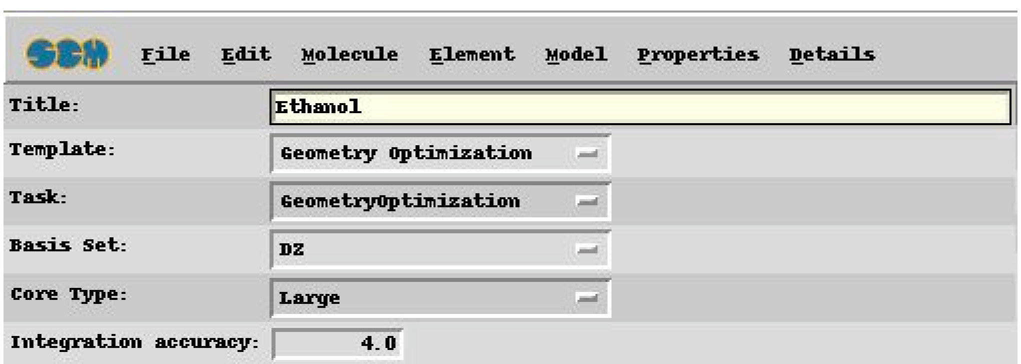
Templates might change any number of input options. In this particular example, only the main Task will change from 'Single Point' to 'Geometry Optimization'.

If you would set the template again later, all input values will revert to the default values and you will loose all your changes!

Title

This field, currently empty, has no special meaning. It will be used as an identifier for your convenience in the result files of the ADF calculation. In this case, lets set the title to the name of the molecule:

`Enter 'Ethanol' without quotes in the 'Title' field.`



Note that as soon as you start typing in the title field, the color of the field changes. This indicates that you have made a change with respect to the value stored in the template for this field.

Task

This is the main task the program will perform. In this case it will optimize the geometry of the molecule.

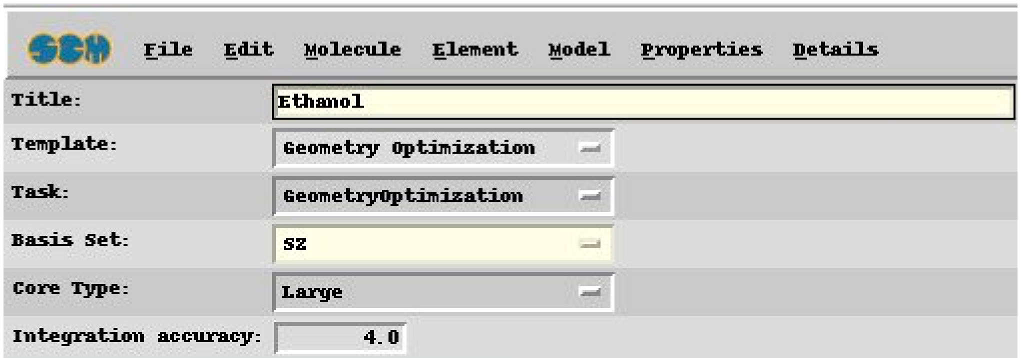
Basis set

With the 'Basis Set' pull-down menu you select the basis set you want to use.

The menu gives access to the basis sets regularly used.

For this tutorial we will choose a very small basis set. This will result in poor results, but the calculation runs much faster. Thus:

```
Select 'SZ' from the 'Basis Set' pull-down menu
```



Core type

With the 'Core Type' pull-down menu you select the kind of core to use. This is really a further specification of the basis set.

For the tutorial a Large core is fine.

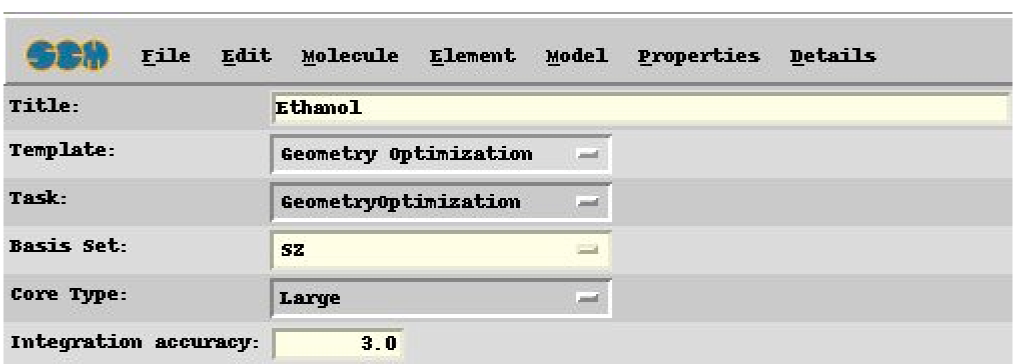
Integration

The ADF software package uses a numerical integration scheme for virtually everything it may calculate. The number specified here is roughly the number of significant digits in your results.

Increasing the number makes the results more accurate, but will require substantially more computation time. Similarly, decreasing the number will result in less accurate results, but you will get the results much quicker.

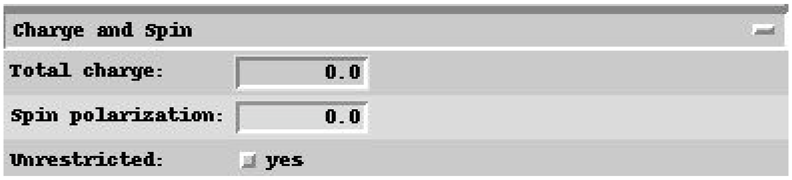
For the tutorial, we will reduce the accuracy in order to speed things up:

```
Change the integration accuracy to 3.0.
```



Charge and Spin

On the right side of the window you will find many more input fields. They are organized in panels. You select a panel with the pull-down menu showing the title of the panel, along the topside.



Alternatively, you can select the panel you are interested in from the main menu (Model, Properties, or Details).

The current panel showing is the 'Charge and Spin' panel. Here you can specify the total charge of your molecule, and the spin polarization.

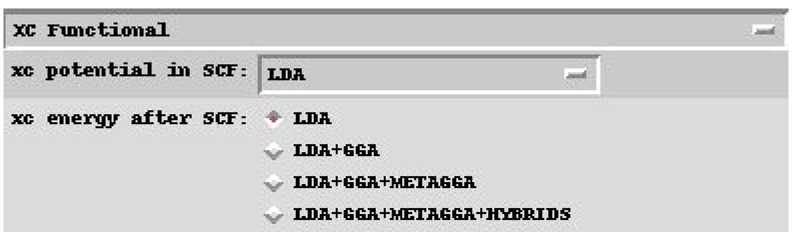
Since ethanol is a closed-shell neutral molecule the default settings are fine.

XC functional

Another important input option is the XC functional to use. To choose the XC functional:

`Select the XC functional`

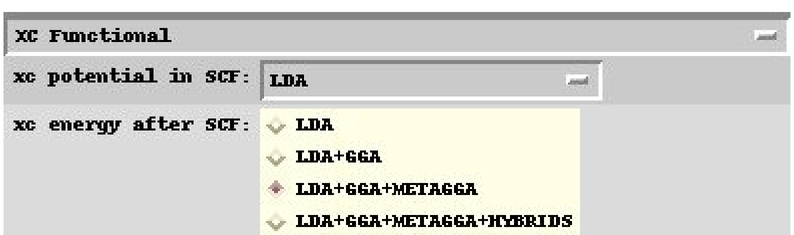
(from the drop down menu, or from the main Model menu).



For this tutorial the default simple (and fast) LDA potential during the SCF is sufficient.

By selecting the LDA+GGA+METAGGA option for the xc energy ADF will print a table at the end of the calculation showing the energies with many different functionals:

`Select the 'LDA+GGA+METAGGA' option for the xc energy after SCF`



Again, since you made a change with respect to the template currently in use the change is highlighted with a yellow color.

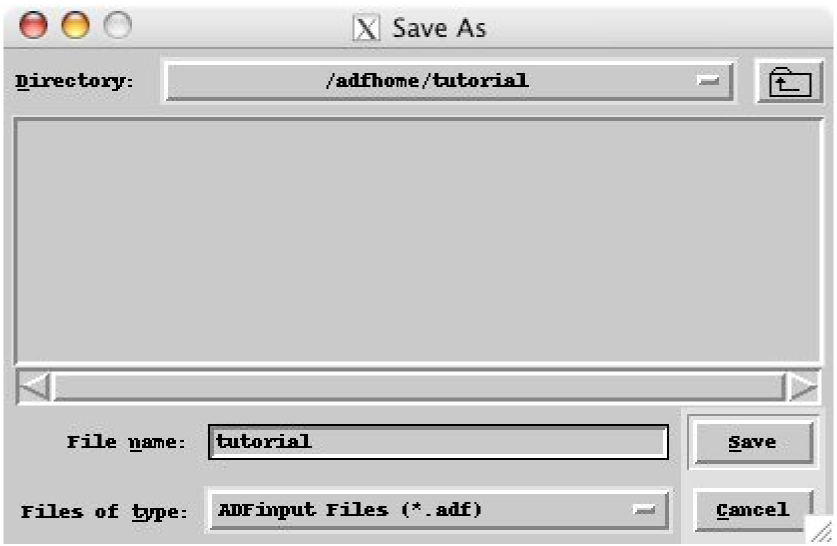
Step 4: Run your calculation

Save your input and create job script

Finally you will want to save your input.

```
Seleect the 'Save' command from the 'File' menu.

Enter the name 'tutorial' in the File name field.
```




```
Click on Save
```

Now you have saved your current options and molecule information. The file will automatically get the extension '.adf'.

ADFinput has also created a corresponding script file, which you can use to start the calculation according to your current input options. This script file has the same name, but with an extension '.run' instead of '.adf'. It also has the execute permission set for the current user.

In your terminal window, check the current files

```
% ls -l
total 24
-rw-r-----  1 visser  admin  5099 14 May 15:27 tutorial.adf
-rwxr-----  1 visser  admin  3082 14 May 15:27 tutorial.run
```

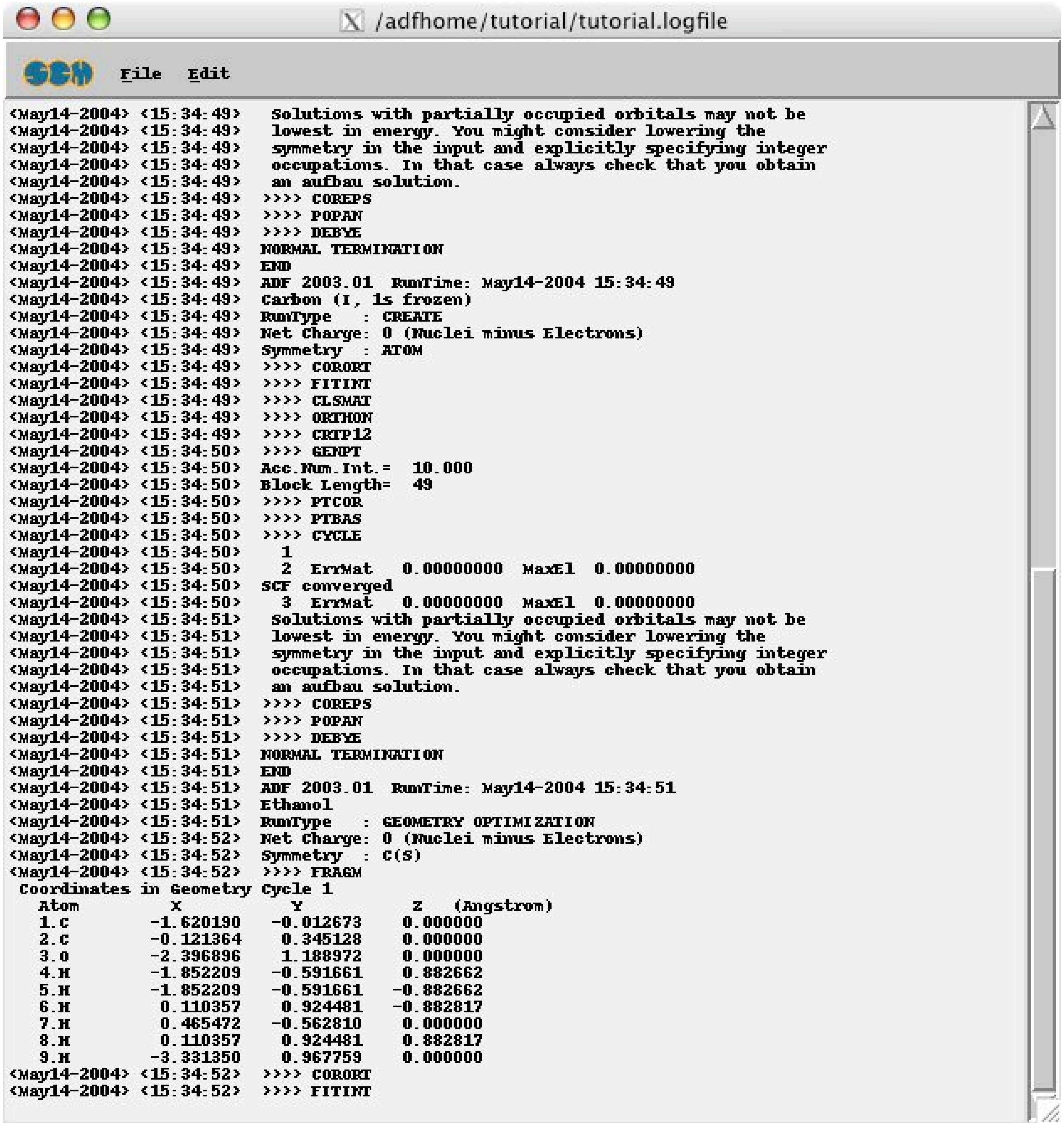
Run your calculation

To actually perform the calculation (thus the geometry optimization of the ethanol molecule), use the Run command from the File menu.

We already saved our changes. If not, the File:Run command will also ask you if it is ok to save the changes.

`Select the 'Run' command from the 'File' menu`

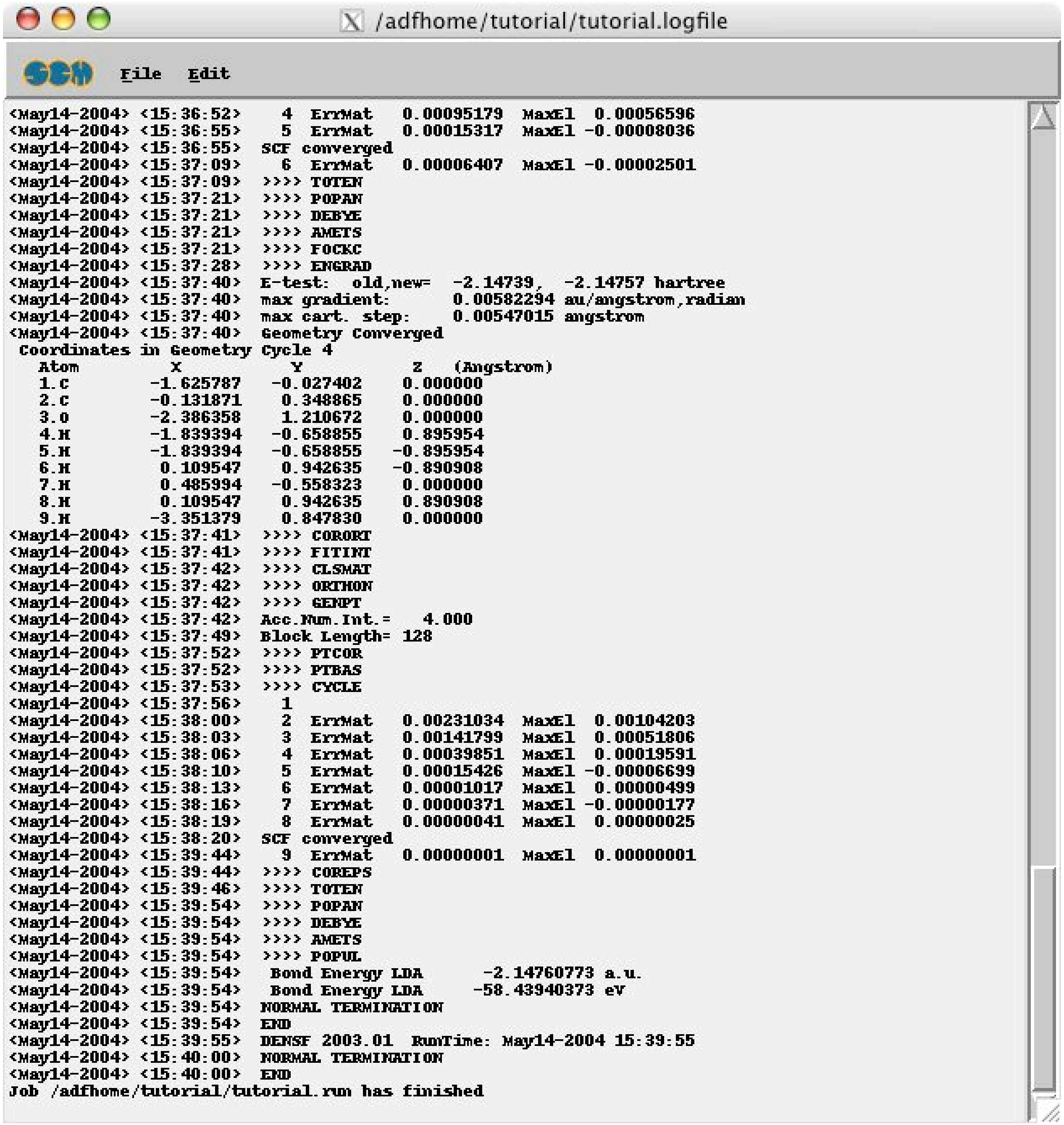
This will execute the run script that has just been created in the background on your local computer. It will also start ADFtail to monitor the progress of the calculation (the logfile):




```
<May14-2004> <15:34:49>   Solutions with partially occupied orbitals may not be
<May14-2004> <15:34:49>   lowest in energy. You might consider lowering the
<May14-2004> <15:34:49>   symmetry in the input and explicitly specifying integer
<May14-2004> <15:34:49>   occupations. In that case always check that you obtain
<May14-2004> <15:34:49>   an aufbau solution.
<May14-2004> <15:34:49>  >>>> COREPS
<May14-2004> <15:34:49>  >>>> POPAN
<May14-2004> <15:34:49>  >>>> DEBYE
<May14-2004> <15:34:49>  NORMAL TERMINATION
<May14-2004> <15:34:49>  END
<May14-2004> <15:34:49>  ADF 2003.01  RunTime: May14-2004 15:34:49
<May14-2004> <15:34:49>  Carbon (I, 1s frozen)
<May14-2004> <15:34:49>  RunType    : CREATE
<May14-2004> <15:34:49>  Net Charge: 0 (Nuclei minus Electrons)
<May14-2004> <15:34:49>  Symmetry   : ATOM
<May14-2004> <15:34:49>  >>>> CORORT
<May14-2004> <15:34:49>  >>>> FITINT
<May14-2004> <15:34:49>  >>>> CLSMAT
<May14-2004> <15:34:49>  >>>> ORTHON
<May14-2004> <15:34:49>  >>>> CRTP12
<May14-2004> <15:34:50>  >>>> GENPT
<May14-2004> <15:34:50>  Acc.Num.Int.=   10.000
<May14-2004> <15:34:50>  Block Length=   49
<May14-2004> <15:34:50>  >>>> PTCOR
<May14-2004> <15:34:50>  >>>> PTBAS
<May14-2004> <15:34:50>  >>>> CYCLE
<May14-2004> <15:34:50>    1
<May14-2004> <15:34:50>    2  ErrMat    0.00000000  MaxEl  0.00000000
<May14-2004> <15:34:50>  SCF converged
<May14-2004> <15:34:50>    3  ErrMat    0.00000000  MaxEl  0.00000000
<May14-2004> <15:34:51>   Solutions with partially occupied orbitals may not be
<May14-2004> <15:34:51>   lowest in energy. You might consider lowering the
<May14-2004> <15:34:51>   symmetry in the input and explicitly specifying integer
<May14-2004> <15:34:51>   occupations. In that case always check that you obtain
<May14-2004> <15:34:51>   an aufbau solution.
<May14-2004> <15:34:51>  >>>> COREPS
<May14-2004> <15:34:51>  >>>> POPAN
<May14-2004> <15:34:51>  >>>> DEBYE
<May14-2004> <15:34:51>  NORMAL TERMINATION
<May14-2004> <15:34:51>  END
<May14-2004> <15:34:51>  ADF 2003.01  RunTime: May14-2004 15:34:51
<May14-2004> <15:34:51>  Ethanol
<May14-2004> <15:34:51>  RunType    : GEOMETRY OPTIMIZATION
<May14-2004> <15:34:52>  Net Charge: 0 (Nuclei minus Electrons)
<May14-2004> <15:34:52>  Symmetry   : C(S)
<May14-2004> <15:34:52>  >>>> FRAGM
 Coordinates in Geometry Cycle 1
   Atom         X           Y           Z    (Angstrom)
   1.C      -1.620190   -0.012673    0.000000
   2.C      -0.121364    0.345128    0.000000
   3.O      -2.396896    1.188972    0.000000
   4.H      -1.852209   -0.591661    0.882662
   5.H      -1.852209   -0.591661   -0.882662
   6.H       0.110357    0.924481   -0.882817
   7.H       0.465472   -0.562810    0.000000
   8.H       0.110357    0.924481    0.882817
   9.H      -3.331350    0.967759    0.000000
<May14-2004> <15:34:52>  >>>> CORORT
<May14-2004> <15:34:52>  >>>> FITINT
```

Step 5: Results of your calculation

`Wait for your calculation to finish:`
`the logfile should end with` **"Job ... has finished"**



It might take a while before the last line appears, depending on the speed of your computer. ADF is very busy optimizing the geometry of ethanol ...

We do not need the logfile any more, so lets close that window.

```
In the window showing the logfile (the ADFtail window):

Select the 'Quit' command from the 'File' menu
```

Now ADF has created a couple of data files and a couple of text files. You can check this in your terminal window:

```
% ls -l
```

```
total 4200
-rw-r-----  1 visser  admin    5099 14 May 15:27 tutorial.adf
-rw-r-----  1 visser  admin     125 14 May 15:40 tutorial.err
-rw-r-----  1 visser  admin   12173 14 May 15:40 tutorial.logfile
-rw-r-----  1 visser  admin  209032 14 May 15:40 tutorial.out
-rwxr-----  1 visser  admin    3082 14 May 15:27 tutorial.run
-rw-------  1 visser  admin   69632 14 May 15:40 tutorial.t13
-rw-------  1 visser  admin  876544 14 May 15:40 tutorial.t21
-rw-------  1 visser  admin  962560 14 May 15:40 tutorial.t41
```

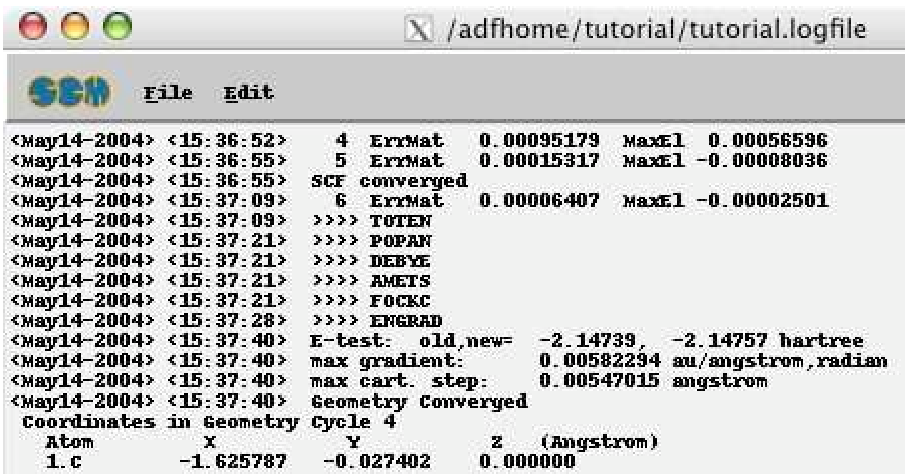
Using the SCM menu (on most systems the SCM logo on the left side of the menu bar, on some systems just the letters 'SCM') you can easily start other parts of the ADF GUI to have a look at your results.

The SCM menu is available on most ADF GUI programs, and you can use it to switch between the active ADF GUI windows as well.

Logfile

As a first example of using the SCM menu, take a look again at the logfile. You have already seen it: while the calculation is running it is shown using the ADFtail module. If you wish to see it again, use the SCM menu:

`Select the 'Logfile' command from the 'SCM' menu (the icon on the left side of the menu bar)`



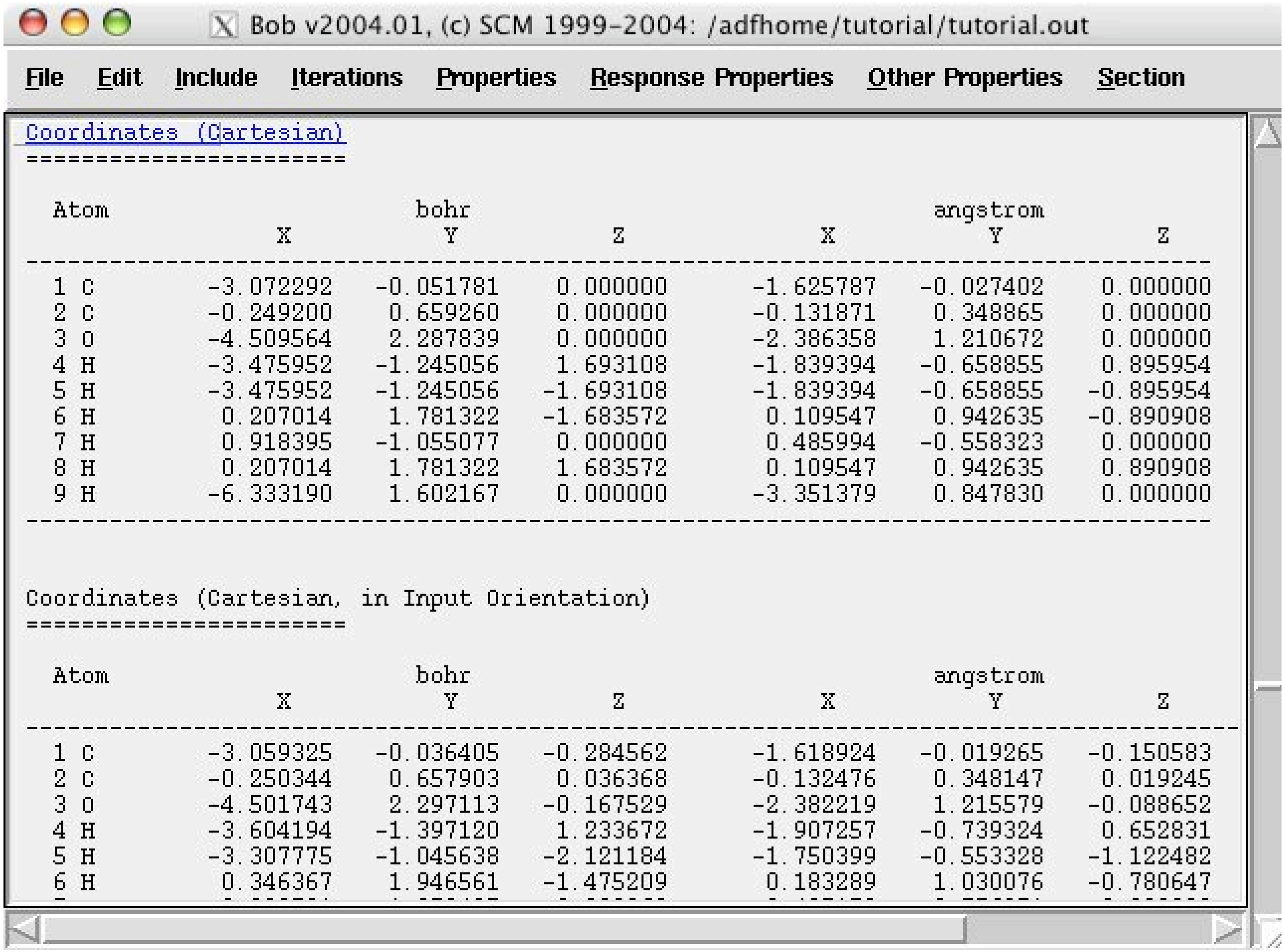
You already know how to close it again, if you wish to do so.

Output

The output file (tutorial.out) is a plain text file. You can view it with your favorite text editor (or text viewer). You can also use the Bob (basic output browser) to have a look at the results:

`Select the 'Output' command from the 'SCM' menu`

The Bob program will start showing the results of your calculation.



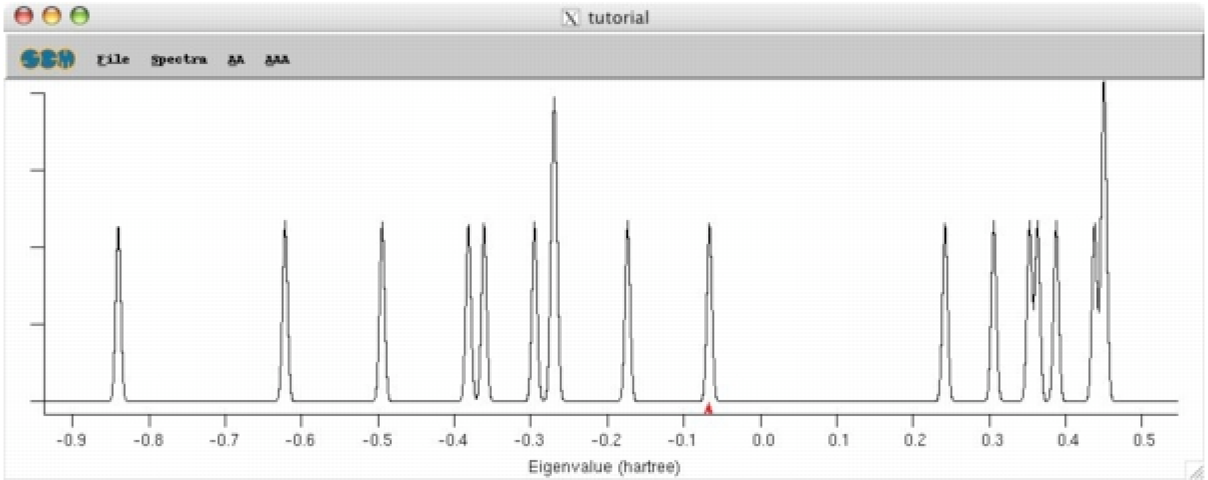
You can use the menus to go to different parts of the output file, or you can just use the scroll bar. Have a look, and then close the program.

```
Select the 'Quit' command from the 'File' menu in the Bob window (showing the output)
```

DOS (density of states)

Part of the results of the calculation is typically a large number of orbital energies. These may be graphically represented as a DOS (density of states). To see this DOS use the ADFspectra utilty:

```
Select the 'Spectra' command from the 'SCM' menu
```



The little red arrow along the horizontal energy axis corresponds to the Fermi level (the highest occupied orbital). The height of the peaks depend on the number of peaks close together (real or accidental degeneracies).

Geometry changes

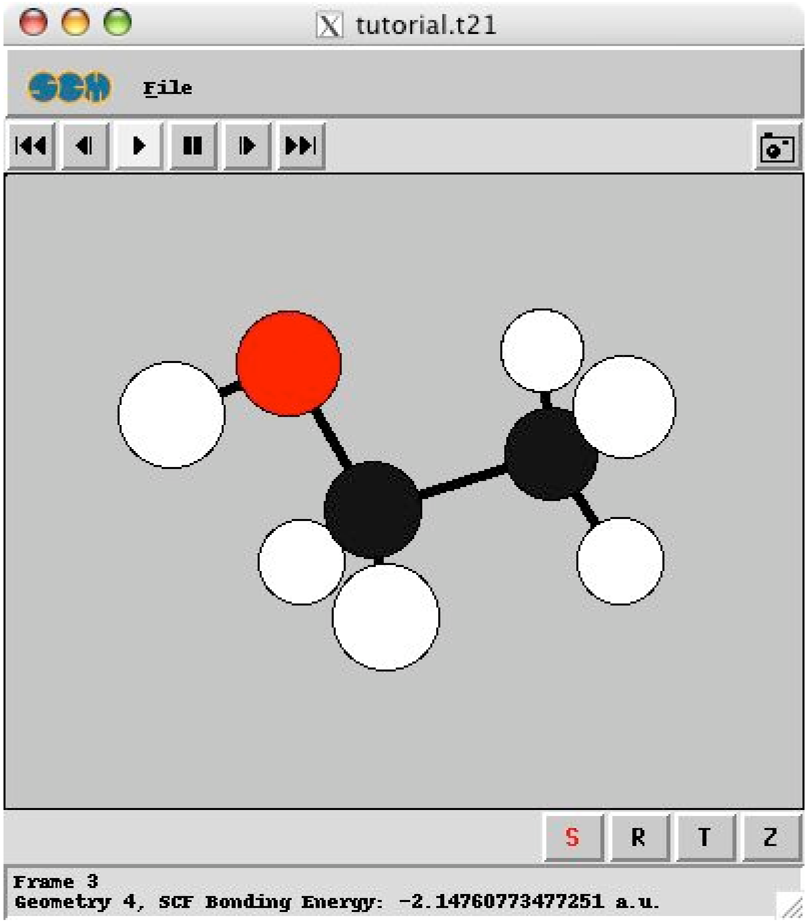
It is very easy to view the change in geometry of the molecule as a result of the geometry optimization by ADF as a small movie:

```
Select the 'Movie' command from the 'SCM' menu
```

```
Rotate the picture with the mouse, just as in ADFinput
```

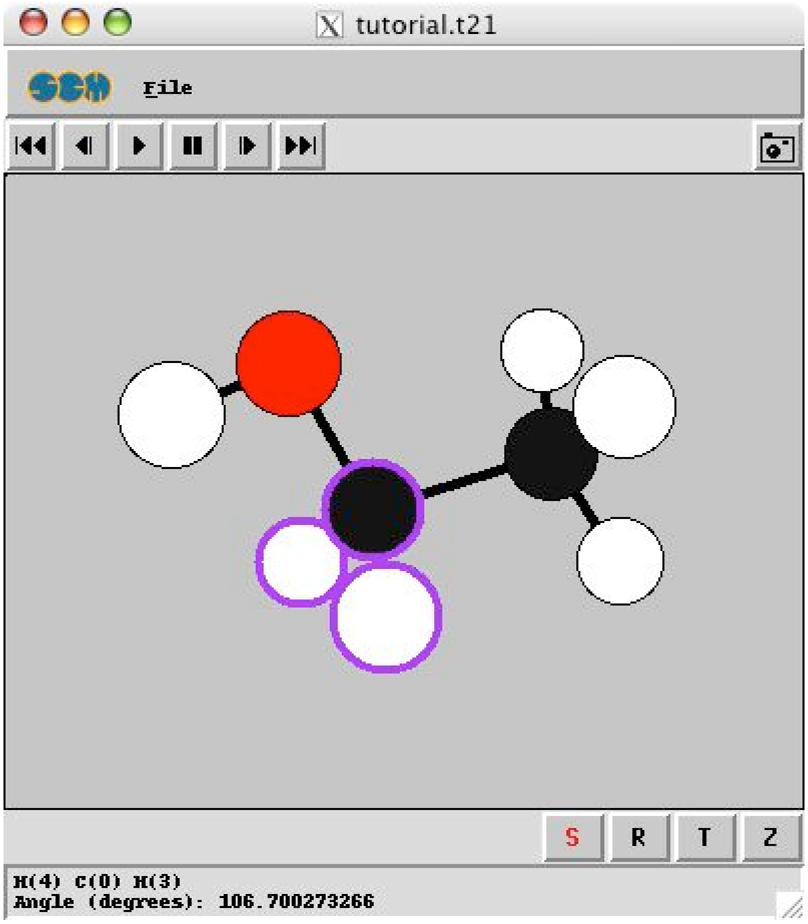
Using the buttons you can replay the movie, or move one frame forwards or backwards.

You can also rotate and zoom etc, exactly as in ADFinput.



By selecting a couple of atoms you can get information about bond distances, angles and dihedrals.

`Select three atoms by shift-clicking`



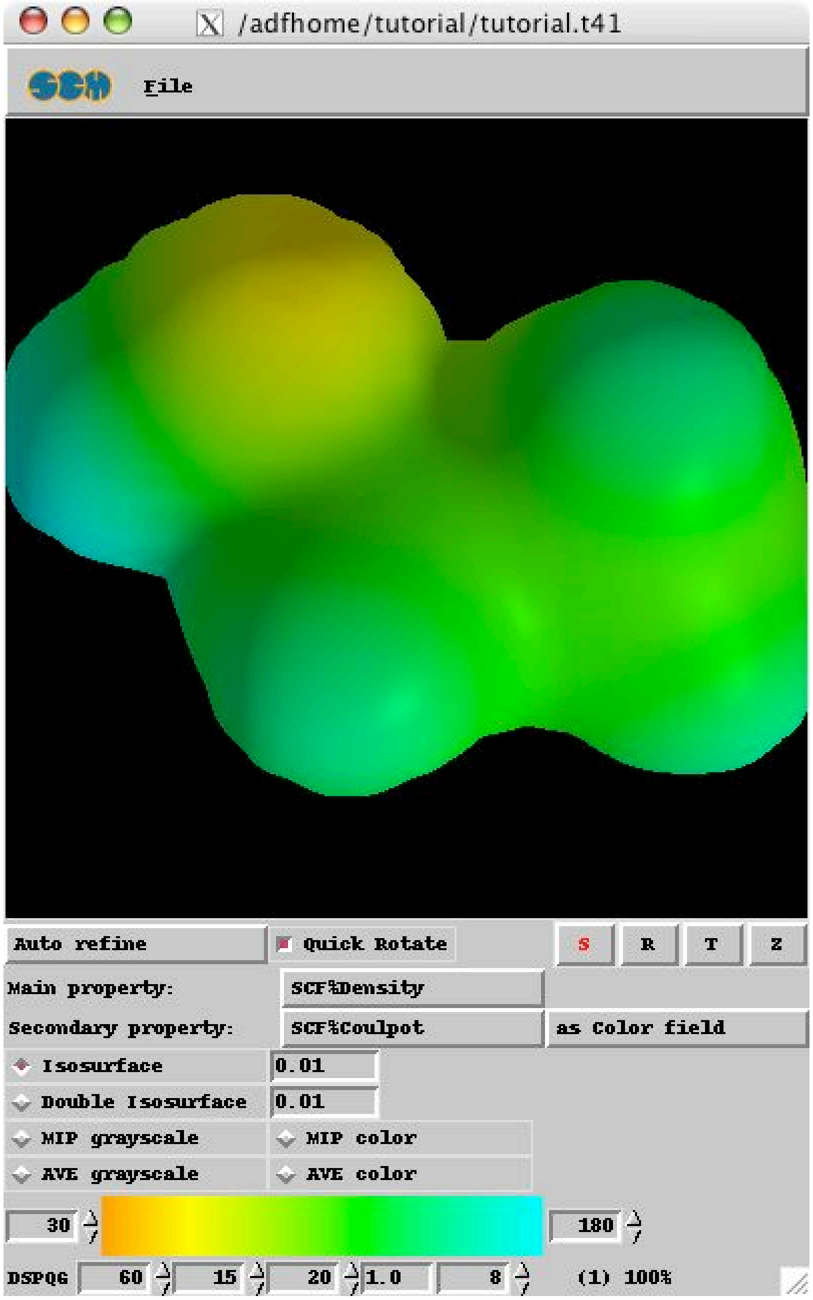
ADFmovie shows all geometries that are available on the tutorial.t21 file. You can also view geometries from a logfile, just open the logfile from the File menu (or start ADFmovie from the command line with the logfile as argument).

Electron density

The final electron density, electrostatic potential and orbitals as calculated by ADF are also available on a grid, in the tutorial.t41 file. This file has actually been created by the densf utility (as you might check in the logfile, at the end of the file).

These 3D data fields may be visualized using ADFview.

```
Select the 'View' command from the 'SCM' menu
```



ADFview will start, showing the final SCF density colored by the electrostatic potential.

ADFview tutorial

This tutorial will help you to visualize volume properties (densities, orbitals, electrostatic potential) in a variety of ways. ADFview needs the values of these fields on grid points of a three-dimensional grid. This is done by running the densf utility program, and is automatically done for you when you use ADFinput to set up your calculation.

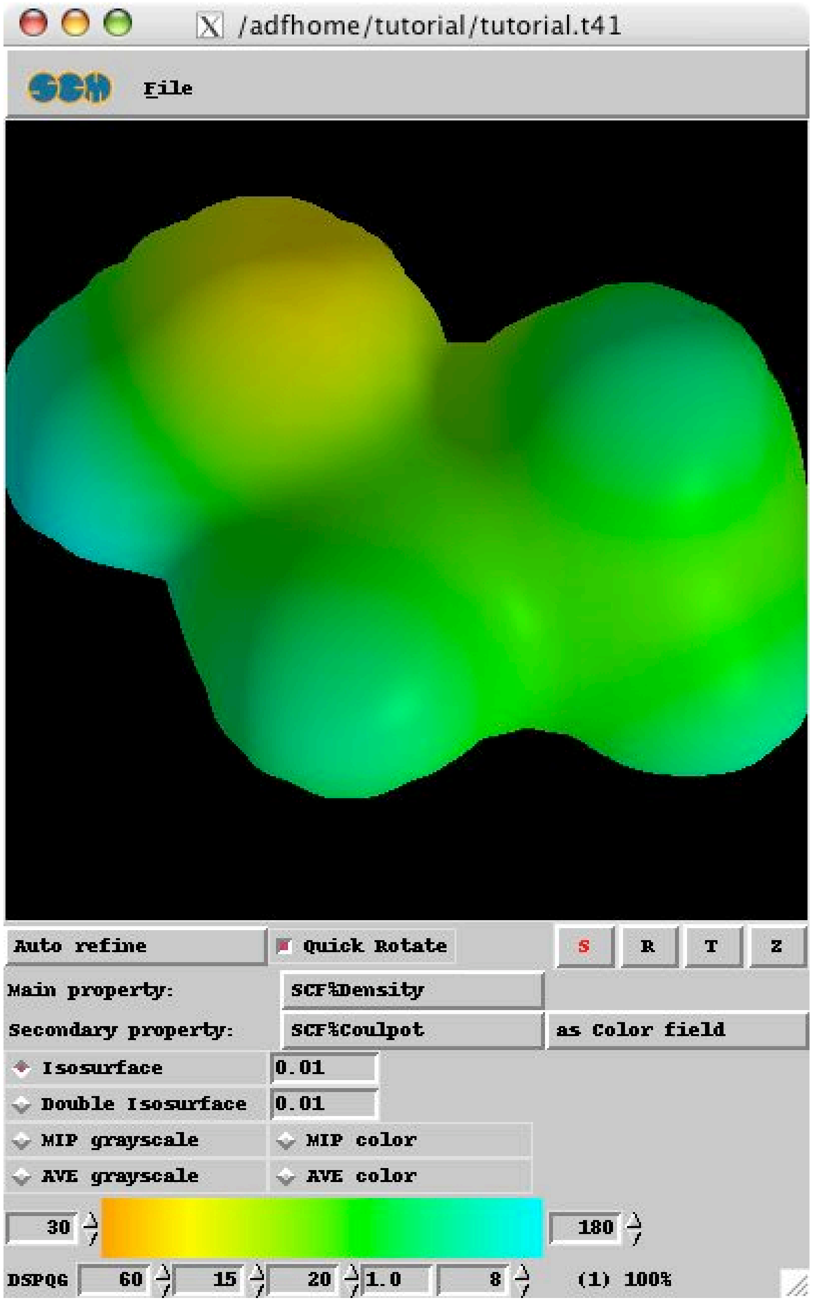
Starting ADFview

In this tutorial we will continue to work with the files that have been generated in the first (ADFinput) tutorial. If ADFview is not running any more, please start it again.

Only when ADFview is not running any more:

```
cd $ADFHOME/tutorial
adfview tutorial.t41
```

A new window will be created on your display. The upper part of this window contains a picture, if available. The lower part contains the controls you use to tell ADFview what to do.



After the computation has finished, the start-up screen shows an isodensity surface of the ethanol molecule, colored according to the values of the Coulomb potential.

Immediately after starting, ADFview will scan the tutorial.t41 as specified on the command line. Next it will load some volume properties from it, and it will start calculating and displaying an image. Please be patient, and let the program continue the calculations until the picture has been created in the best possible quality.

In the lower right corner of the ADFview window you can see if the picture is complete. The number in parentheses is an indication of the quality of the picture being calculated, with 1 being the best quality. The percentage value is the part of the calculations completed.

This image is an isosurface of the SCF density, and has been colored with the electrostatic potential. Later in this tutorial we will show you how to generate different pictures. The isosurface value is 0.01. You can change that by simply changing the number to the right of 'Isosurface'.

Play around with the color range

You can change the color range used to indicate different values of the electrostatic potential. The entire range of the electrostatic potential values is mapped on the color range visible in the horizontal color bar. You can change this bar:

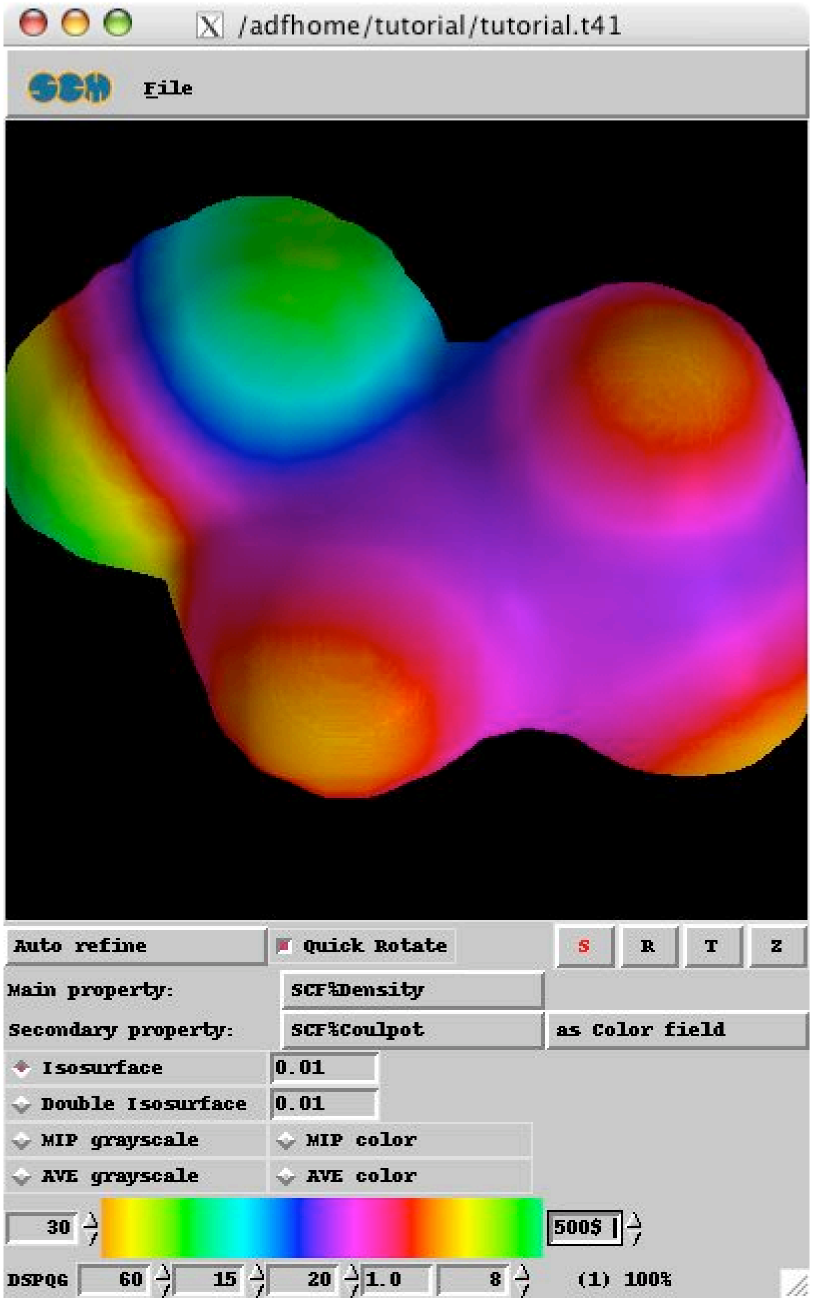
```
Click on the little arrows next to the color bar
```

The image as well as the color bar will update immediately. You can also change the color range by changing the numbers on the left and right side of the bar:

```
Select the right number by double-clicking on it.

Type a new value (500)

Press the Return key
```



Again, the picture and color bar will update immediately.

Rotate the image

The following instructions assume you are using a three-button mouse. If you have a mouse with one or two buttons, check the description of the S, R, T, and Z buttons in the reference manual to learn how to achieve the same effects.

```
Click in the picture and hold down the right mouse button
```

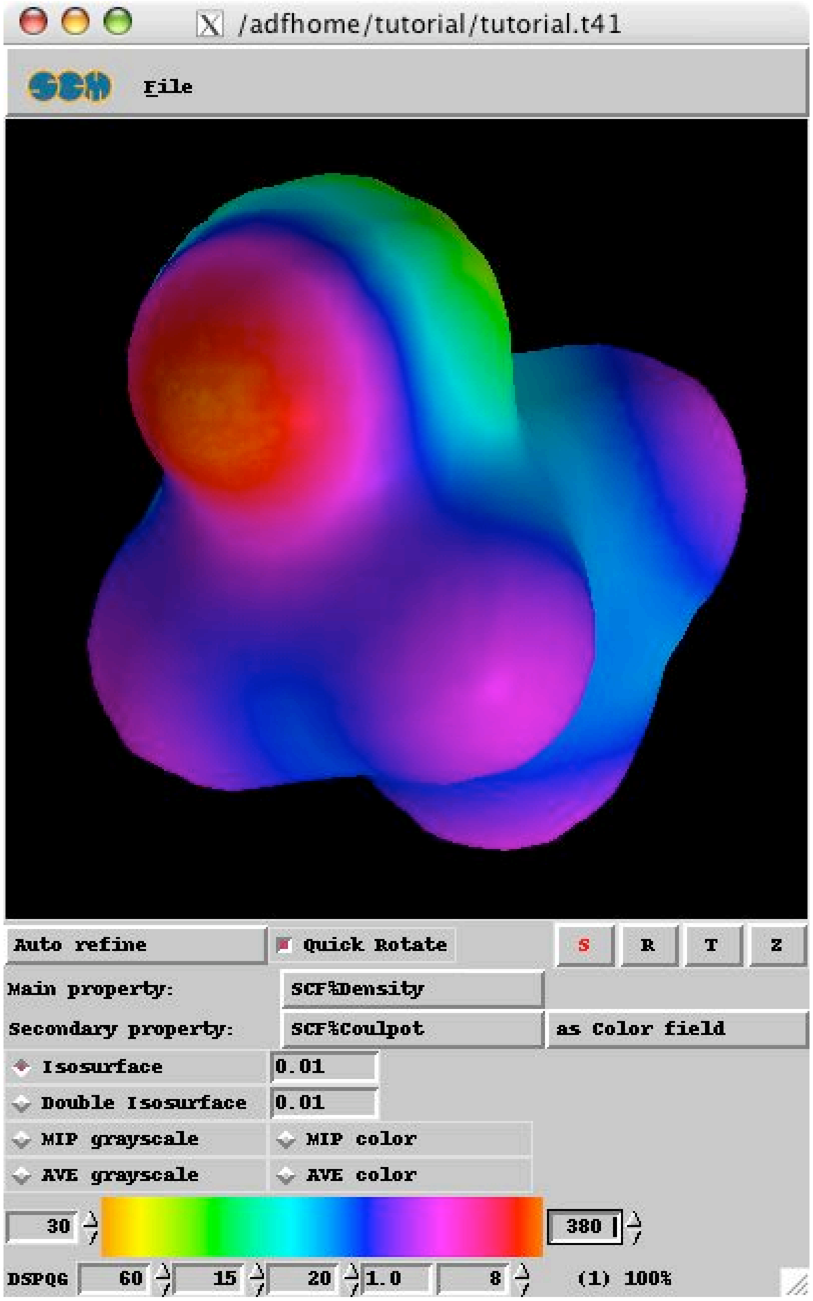
The picture will change into a diagram of the ethanol molecule, inside a cube.

```
Move the mouse around (still pressing the right mouse button!)
```

The picture of the ethanol molecule and the cube will rotate.

`Release the mouse button`

The picture of the ethanol molecule and the cube will disappear, and ADFview will recalculate the isosurface of the density in the new orientation.



Rotating works using a 'virtual trackball': when you move the mouse somewhere in the center, the picture changes as if you were rotating by pushing the top of the ball. If you move the mouse near the edge of the picture (outside the rectangle), the rotation will be around an axis perpendicular to the screen.

Zoom the image

```
Press and hold the control key, click in the picture and hold
down the right mouse button
```

The picture will change to a ethanol molecule in a simple cube.

```
Move the mouse to the right (still pressing the right mouse
button and control key!)
```

As the picture of the cube and the molecule shows, you will zoom in.

```
Move the mouse to the left (still pressing the right mouse
button and control key!)
```

You will zoom out.

```
Release the mouse button
```

The cube and molecule will disappear, and ADFview will recalculate the isosurface of the density with the new zoom settings.

Translate the image

```
Click in the picture using the middle mouse button, and hold
down the mouse button
```

```
Drag the mouse in some direction
```

The image (temporarily replaced by the picture of the cube) will be translated following the mouse.

Remove electrostatic potential coloring

Click on 'as Color Field' and hold the mouse button down

A menu will appear. This menu tells you how ADFview is using the 'secondary property' selected (currently the electrostatic potential).

```
Select the '- not used -' entry
```

A simple grayscale picture of the isosurface of the SCF density will replace the image.

View an orbital

```
Click on 'SCF%Density' and hold the mouse button down
```

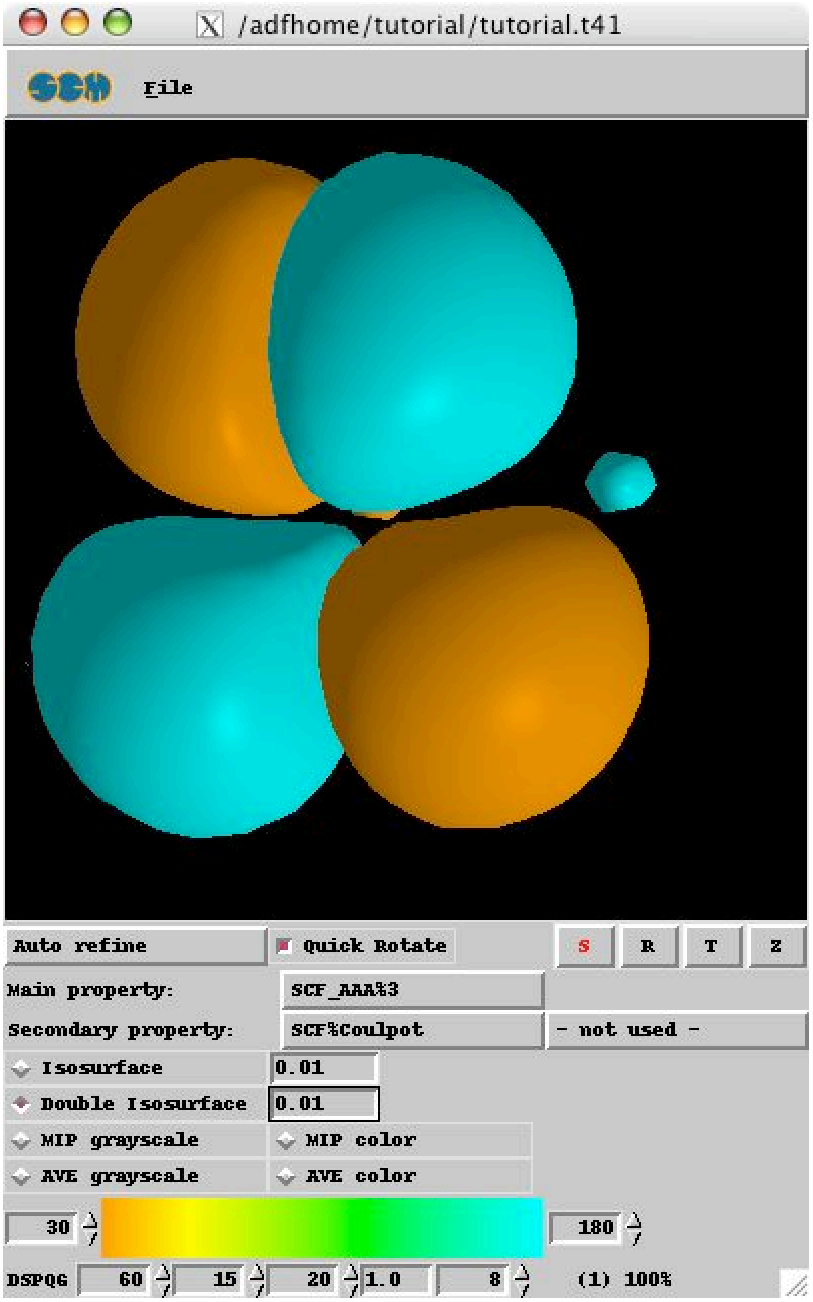
A menu will appear. This menu lists all volume properties available on tutorial.t41.

```
Select the 'SCF_AAA%3' entry
```

This is the 3rd orbital in the AAA representation, in this case the HOMO within the AAA representation. It is easy to check this by having a look at the menus in ADFspectra with the DOS of ethanol.

The image will change but is not quite optimal. So:

```
Click on 'Double Isosurface'
```



Now a double isosurface should appear. One isosurface corresponds to an isosurface value of 0.01. The other one with a different color corresponds to a value of -0.01. The color on the left side of the color bar is used for the negative isosurface, the color on the right side of the color bar is used for the positive isosurface.

View a difference field

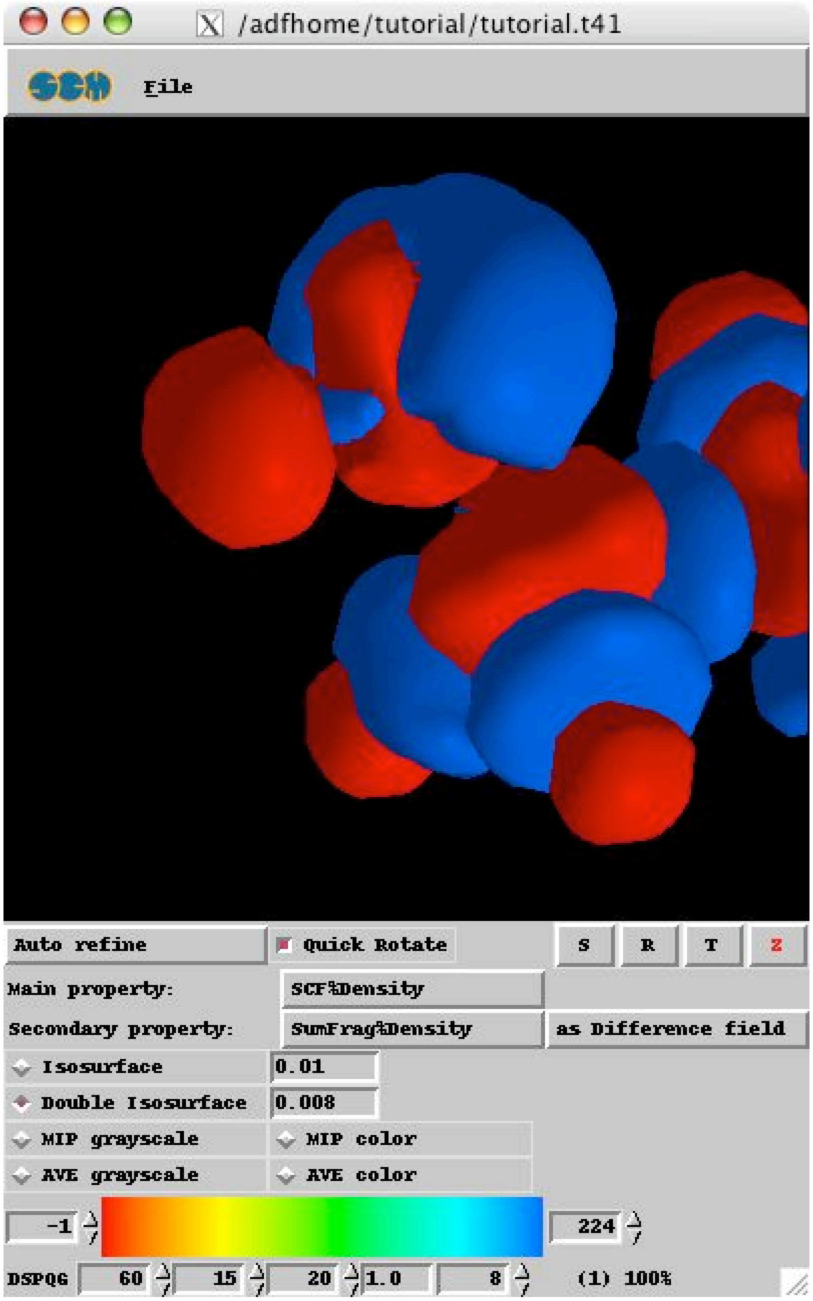
```
Select 'SCF%density' as main property
```

```
Select 'SumFrag%Density' as secondary property
```

```
Change '- not used -' to 'as Difference field'
```

```
Select the 'Double Isosurface' option

Set the number next to 'Double Isosurface' to 0.008
```



These isosurfaces show the difference density between the final SCF density, and the sum of fragments density. Loosely speaking, it shows you how the density changes when building the ethanol molecule from the atomic fragments.

A positive value means that the main property is larger than the secondary property.

View the positive or negative part of a difference field

```
Change 'as Difference field' to 'as Neg Diff field'
```

```
Select Isosurface
```

```
Change the isosurface value to 0.004
```

Now you are viewing the negative part of the difference between the SCF density and the sum of fragments density. The values have been negated to get a positive field.

```
Change 'as Neg Diff field' to 'as Pos Diff field'
```

Now you are viewing the positive part of the same difference field.

View a MIP grayscale image of the density

```
Select 'SCF%Density' as main property
```

```
Select '- not used -' as option with the secondary property
```

```
Select the 'MIP grayscale' mode
```

Now you see an image that looks very much like a 'Röntgen picture' of the molecule. You can clearly see the oxygen atom as well as the carbon and hydrogen atoms.

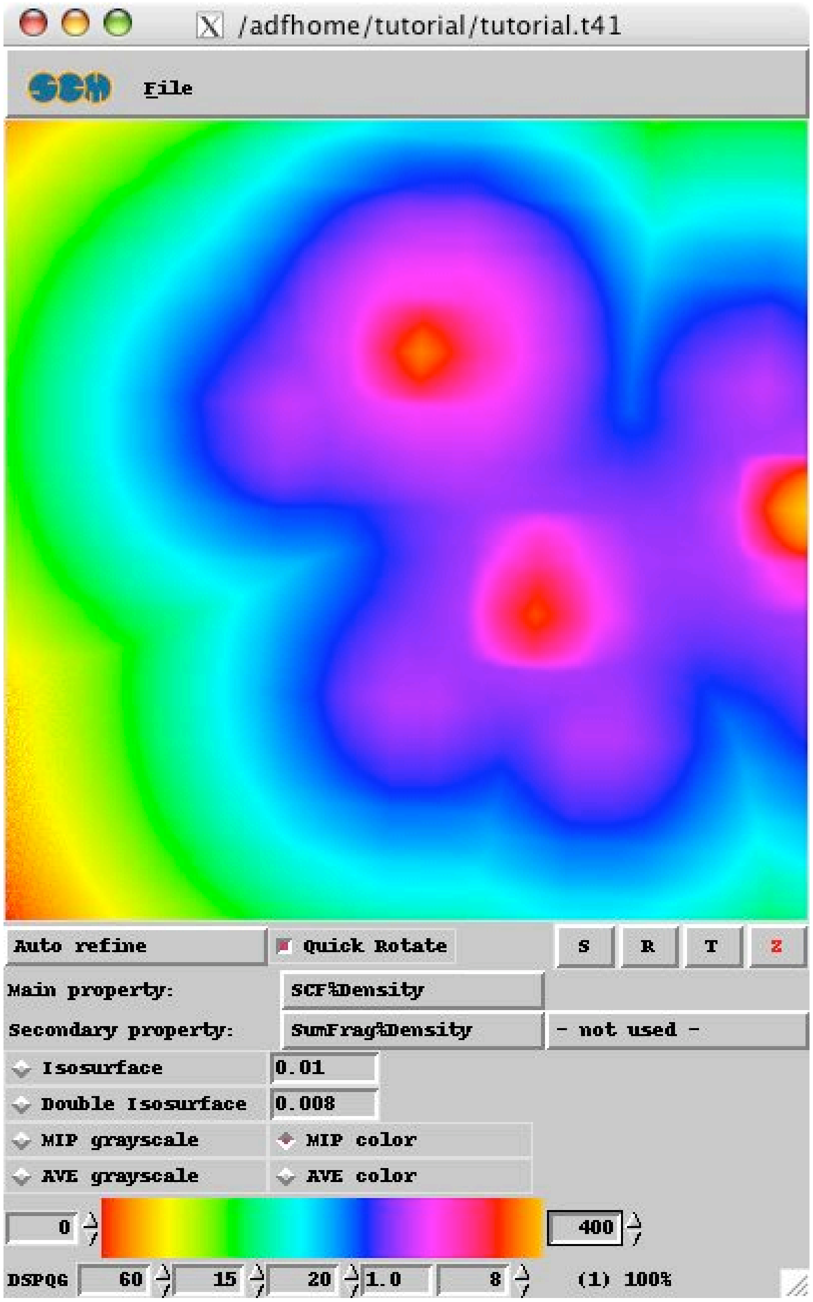
MIP stands for Maximum Intensity Projection. Thus, the image is constructed by sending 'rays' through the data set, and the maximum value encountered determines the intensity at that point of the image.

The nice thing about these pictures is that you can see most of the features in your molecule. The problem is that you do not get a feeling of the three-dimensional structure of it. Of course you can still rotate, and 'take the Röntgen picture from a different angle'.

View MIP color image

```
Select the 'MIP color' mode
```

You will get a similar picture in color.



By playing with the color scale (the horizontal color bar again) you can choose colors which make the features you are interested in better visible. By choosing a large color range (for example from 0 to 1000) you will see many details but in a very busy picture.

Save picture to file

`Select the 'Save As PS' command from the 'File' menu.`

A standard file select dialog box will appear.

Use it to tell ADFview where to save a postscript file with a screen shot of the current picture.

ADFspectra tutorial

This tutorial will show you how to use ADFspectra to visualize some spectra calculated by ADF.

At this point in time the functionality is rather limited: only IR, excitations and DOS spectra are available. No export options, and also no possibilities to change peak shape or width. Such features will probably follow in a later release.

This part of the tutorial does not use the previous examples, so if you still have some ADFGUI programs running you may quit them now.

```
Quit all running ADFGUI programs
```

Part 1: IR spectrum

Create an optimized water molecule

Change to your tutorial directory and start ADFinput:

```
cd $ADFHOME/tutorial
adfinput &
```

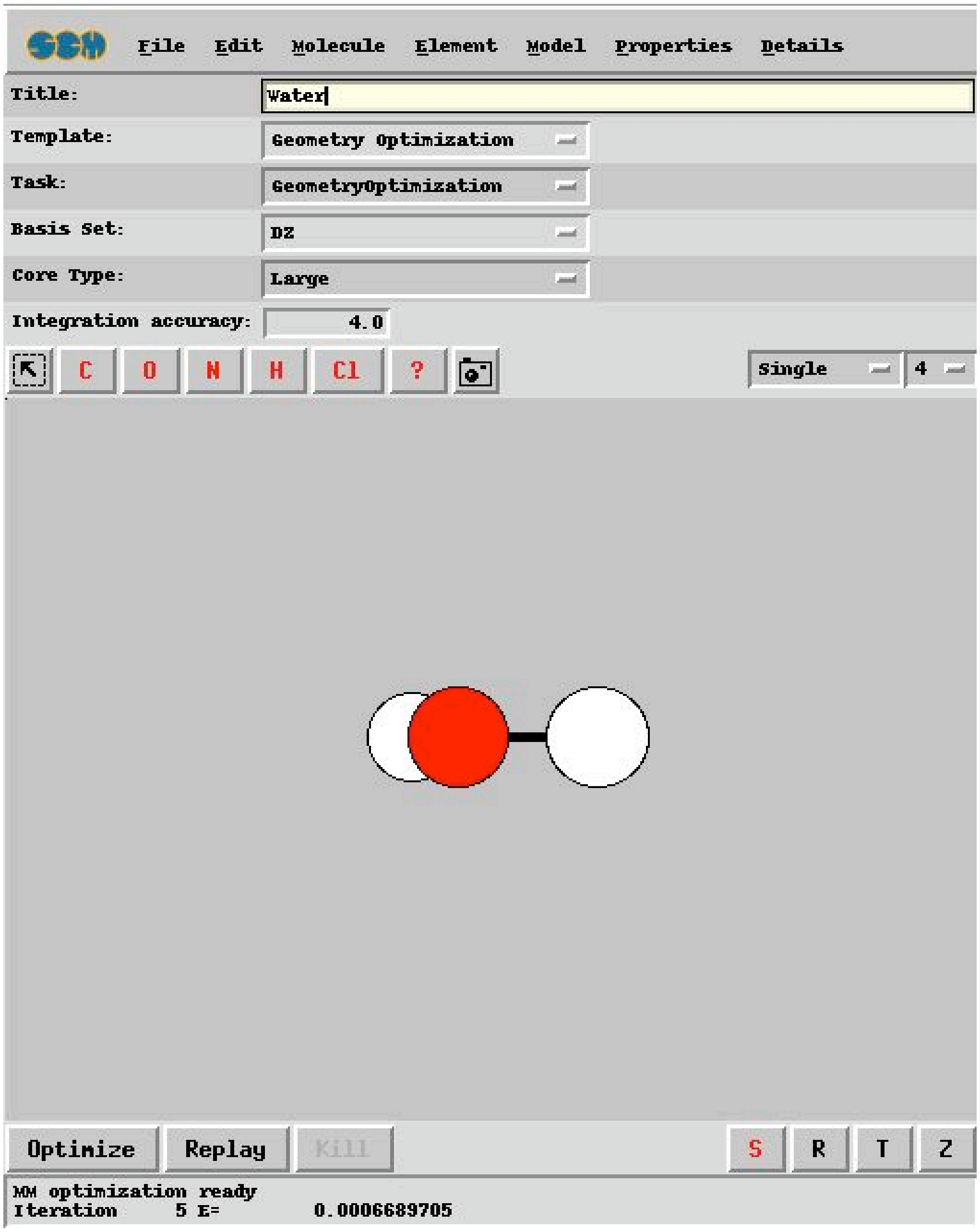
For the IR-spectrum example we will use a rather small molecule: water. So we start with making a water molecule:

```
Select the Oxygen tool
Create one oxygen atom (click once in the empty drawing window)
Select the 'Add Hydrogen' command from the 'Molecule' menu
Click the 'Optimize' button
```

Before doing the actual calculation of the IR frequencies we will optimize the geometry of the water molecule using ADF:

```
Select the 'Geometry Optimization' template
In the Title field, enter 'water'
```

You should now have something very similar to the following:



Now run the calculation:

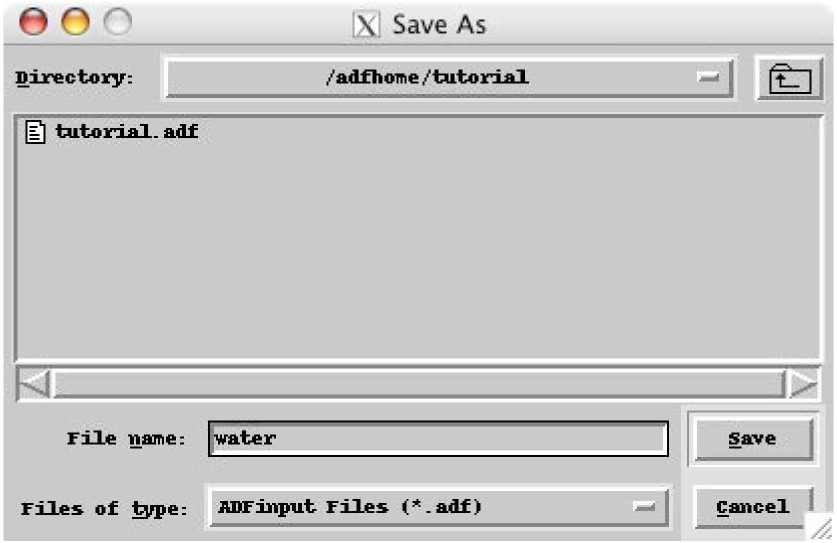
`Select the 'Run' command from the 'File' menu`

The following box will appear:



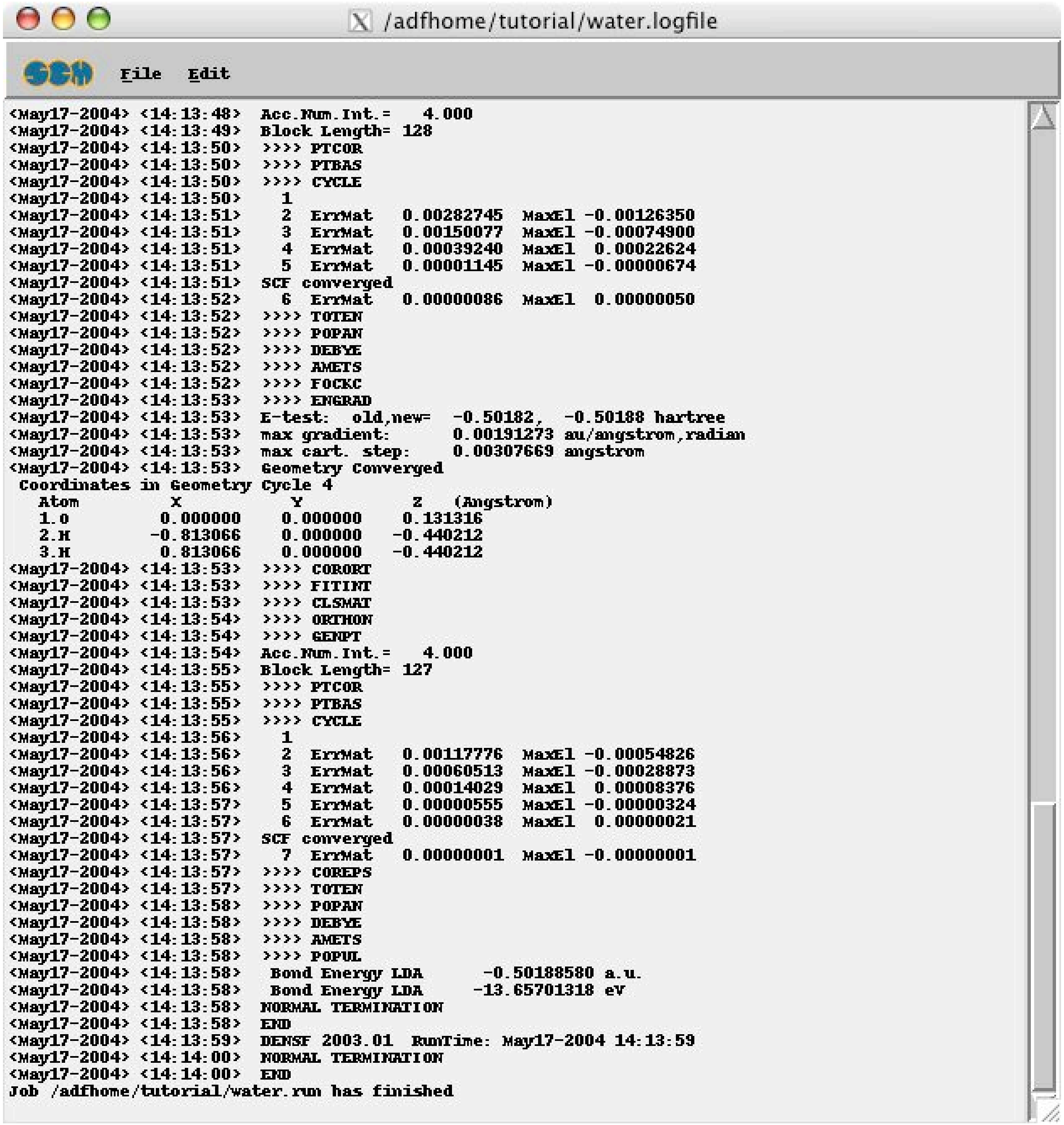
`Click the 'Yes' button to save the setup`

```
Enter 'water' as File name in the Save dialog box
```




```
Click 'Save'
```

Now the geometry optimization of water should start. As in the previous tutorial, a window (ADFtail) showing the contents of the logfile should appear. Wait for the optimization to finish:



```
/adfhome/tutorial/water.logfile
File  Edit
<May17-2004> <14:13:48>  Acc.Num.Int.=   4.000
<May17-2004> <14:13:49>  Block Length= 128
<May17-2004> <14:13:50>  >>>> PTCOR
<May17-2004> <14:13:50>  >>>> PTBAS
<May17-2004> <14:13:50>  >>>> CYCLE
<May17-2004> <14:13:50>    1
<May17-2004> <14:13:51>    2  ErrMat   0.00282745  MaxEl -0.00126350
<May17-2004> <14:13:51>    3  ErrMat   0.00150077  MaxEl -0.00074900
<May17-2004> <14:13:51>    4  ErrMat   0.00039240  MaxEl  0.00022624
<May17-2004> <14:13:51>    5  ErrMat   0.00001145  MaxEl -0.00000674
<May17-2004> <14:13:51>  SCF converged
<May17-2004> <14:13:52>    6  ErrMat   0.00000086  MaxEl  0.00000050
<May17-2004> <14:13:52>  >>>> TOTEN
<May17-2004> <14:13:52>  >>>> POPAN
<May17-2004> <14:13:52>  >>>> DEBYE
<May17-2004> <14:13:52>  >>>> AMETS
<May17-2004> <14:13:52>  >>>> FOCKC
<May17-2004> <14:13:53>  >>>> ENGRAD
<May17-2004> <14:13:53>  E-test:  old,new=  -0.50182,  -0.50188 hartree
<May17-2004> <14:13:53>  max gradient:       0.00191273 au/angstrom,radian
<May17-2004> <14:13:53>  max cart. step:     0.00307669 angstrom
<May17-2004> <14:13:53>  Geometry Converged
 Coordinates in Geometry Cycle 4
   Atom        X           Y           Z    (Angstrom)
   1.O        0.000000    0.000000    0.131316
   2.H       -0.813066    0.000000   -0.440212
   3.H        0.813066    0.000000   -0.440212
<May17-2004> <14:13:53>  >>>> CORORT
<May17-2004> <14:13:53>  >>>> FITINT
<May17-2004> <14:13:53>  >>>> CLSMAT
<May17-2004> <14:13:54>  >>>> ORTHON
<May17-2004> <14:13:54>  >>>> GENPT
<May17-2004> <14:13:54>  Acc.Num.Int.=   4.000
<May17-2004> <14:13:55>  Block Length= 127
<May17-2004> <14:13:55>  >>>> PTCOR
<May17-2004> <14:13:55>  >>>> PTBAS
<May17-2004> <14:13:55>  >>>> CYCLE
<May17-2004> <14:13:56>    1
<May17-2004> <14:13:56>    2  ErrMat   0.00117776  MaxEl -0.00054826
<May17-2004> <14:13:56>    3  ErrMat   0.00060513  MaxEl -0.00028873
<May17-2004> <14:13:56>    4  ErrMat   0.00014029  MaxEl  0.00008376
<May17-2004> <14:13:57>    5  ErrMat   0.00000555  MaxEl -0.00000324
<May17-2004> <14:13:57>    6  ErrMat   0.00000038  MaxEl  0.00000021
<May17-2004> <14:13:57>  SCF converged
<May17-2004> <14:13:57>    7  ErrMat   0.00000001  MaxEl -0.00000001
<May17-2004> <14:13:57>  >>>> COREPS
<May17-2004> <14:13:57>  >>>> TOTEN
<May17-2004> <14:13:58>  >>>> POPAN
<May17-2004> <14:13:58>  >>>> DEBYE
<May17-2004> <14:13:58>  >>>> AMETS
<May17-2004> <14:13:58>  >>>> POPUL
<May17-2004> <14:13:58>   Bond Energy LDA      -0.50188580 a.u.
<May17-2004> <14:13:58>   Bond Energy LDA     -13.65701318 eV
<May17-2004> <14:13:58>  NORMAL TERMINATION
<May17-2004> <14:13:58>  END
<May17-2004> <14:13:59>  DENSF 2003.01  RunTime: May17-2004 14:13:59
<May17-2004> <14:14:00>  NORMAL TERMINATION
<May17-2004> <14:14:00>  END
Job /adfhome/tutorial/water.run has finished
```

Next close the ADFtail window showing the logfile, it is not needed any more:

```
Select the 'Quit' command from the 'File' menu in the window showing the logfile
```

We want to update the coordinates of the water molecule in ADFinput with the optimized coordinates from the ADF calculation. You can do this by closing ADFinput, start it again and read the water.adf file. Easier (and exactly the same result) is to use the Revert command:

```
Select the 'Revert' command from the 'File' menu
```



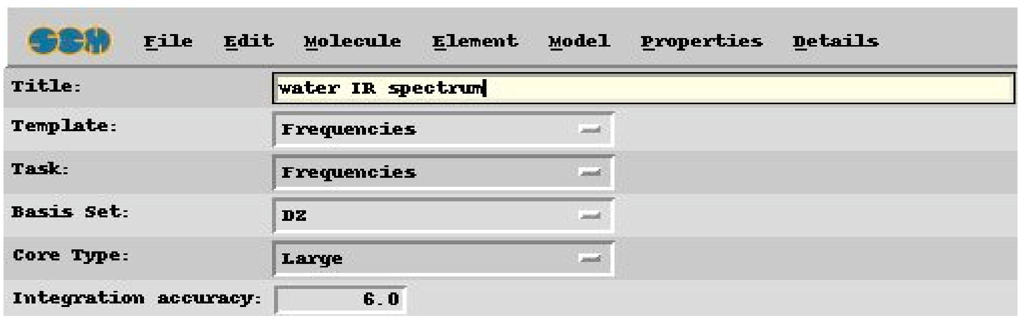

```
Click 'Yes' to use the (ADF-)optimized coordinates
Select the 'Save' command from the 'File' menu
```

So after the last Save command we now have a water molecule, with an optimized geometry corresponding to the current basis set. This is setup is saved in the file water.adf

Perform a frequency calculation

The next step is to calculate the IR frequencies. The only change we need to make is to change the template to Frequencies:

```
Change the template to 'Frequencies'
Change the title to 'Water IR spectrum'
```

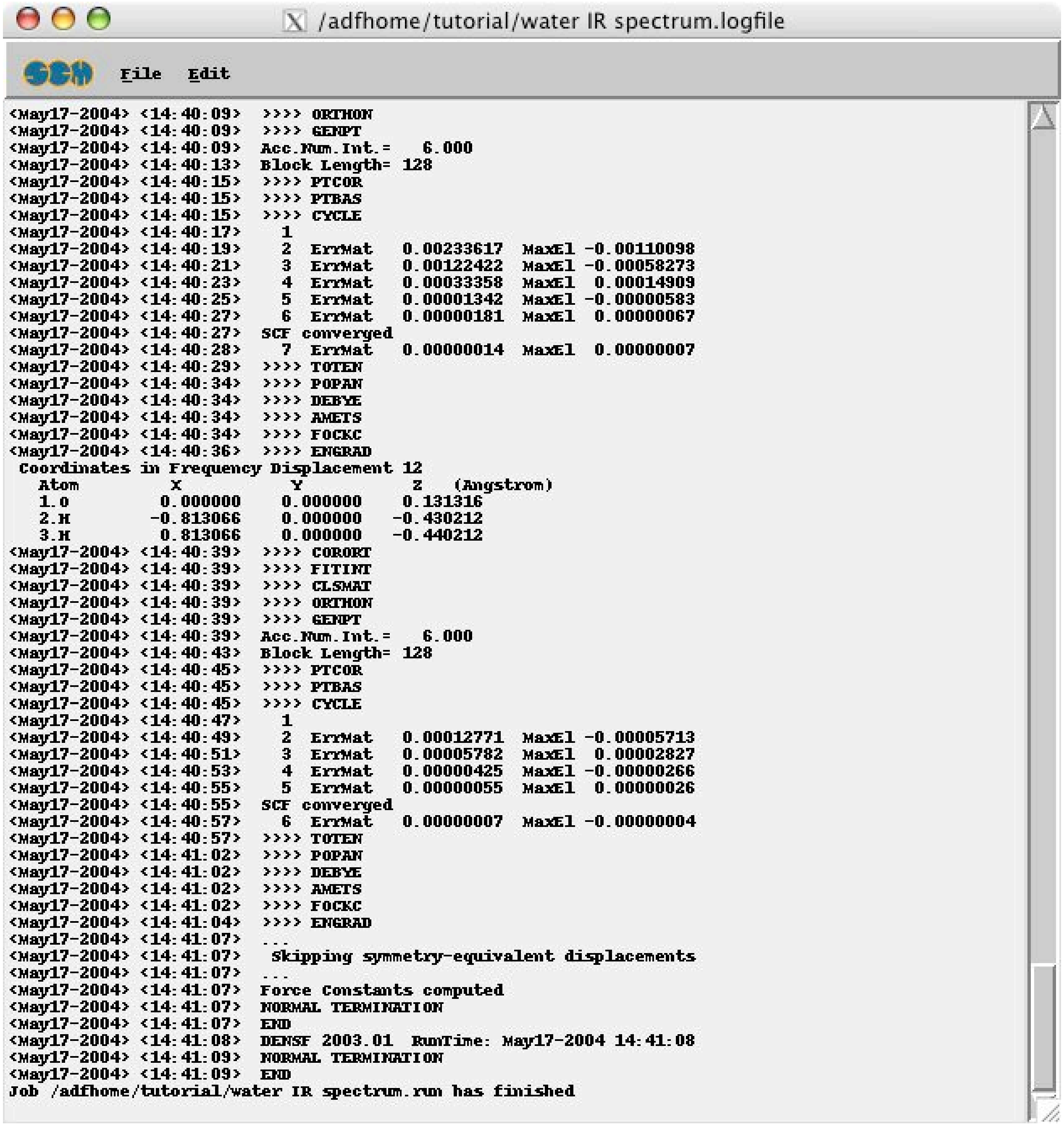


Notice that the default integration accuracy has changed to 6.0. This is required to perform a frequency calculation with accurate results.

Now lets save this input in a different file, and run the calculation:

```
Select the 'Save As...' command from the 'File' menu
Enter 'Water IR spectrum' as file name
Click the 'Save' button
Select the 'Run command from the 'File' menu
```

As you probably expected, a window showing the progress of the calculation (the logfile) pops up. Frequency calculations are relatively time-consuming, so take a up of coffee while waiting for the calculation to finish.

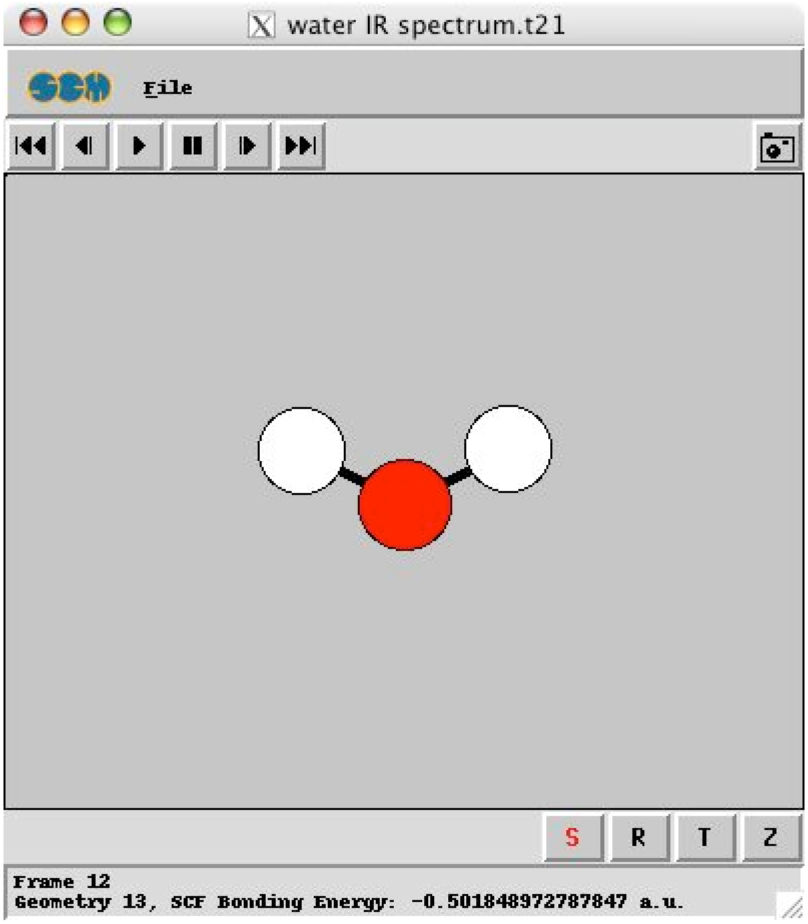

/adfhome/tutorial/water IR spectrum.logfile

File Edit

```
<May17-2004> <14:40:09>  >>>> ORTHON
<May17-2004> <14:40:09>  >>>> GENPT
<May17-2004> <14:40:09>  Acc.Num.Int.=    6.000
<May17-2004> <14:40:13>  Block Length= 128
<May17-2004> <14:40:15>  >>>> PTCOR
<May17-2004> <14:40:15>  >>>> PTBAS
<May17-2004> <14:40:15>  >>>> CYCLE
<May17-2004> <14:40:17>     1
<May17-2004> <14:40:19>     2  ErrMat    0.00233617  MaxEl -0.00110098
<May17-2004> <14:40:21>     3  ErrMat    0.00122422  MaxEl -0.00058273
<May17-2004> <14:40:23>     4  ErrMat    0.00033358  MaxEl  0.00014909
<May17-2004> <14:40:25>     5  ErrMat    0.00001342  MaxEl -0.00000583
<May17-2004> <14:40:27>     6  ErrMat    0.00000181  MaxEl  0.00000067
<May17-2004> <14:40:27>  SCF converged
<May17-2004> <14:40:28>     7  ErrMat    0.00000014  MaxEl  0.00000007
<May17-2004> <14:40:29>  >>>> TOTEN
<May17-2004> <14:40:34>  >>>> POPAN
<May17-2004> <14:40:34>  >>>> DEBYE
<May17-2004> <14:40:34>  >>>> AMETS
<May17-2004> <14:40:34>  >>>> FOCKC
<May17-2004> <14:40:36>  >>>> ENGRAD
 Coordinates in Frequency Displacement 12
   Atom          X           Y           Z    (Angstrom)
   1.O         0.000000    0.000000    0.131316
   2.H        -0.813066    0.000000   -0.430212
   3.H         0.813066    0.000000   -0.440212
<May17-2004> <14:40:39>  >>>> CORORT
<May17-2004> <14:40:39>  >>>> FITINT
<May17-2004> <14:40:39>  >>>> CLSMAT
<May17-2004> <14:40:39>  >>>> ORTHON
<May17-2004> <14:40:39>  >>>> GENPT
<May17-2004> <14:40:39>  Acc.Num.Int.=    6.000
<May17-2004> <14:40:43>  Block Length= 128
<May17-2004> <14:40:45>  >>>> PTCOR
<May17-2004> <14:40:45>  >>>> PTBAS
<May17-2004> <14:40:45>  >>>> CYCLE
<May17-2004> <14:40:47>     1
<May17-2004> <14:40:49>     2  ErrMat    0.00012771  MaxEl -0.00005713
<May17-2004> <14:40:51>     3  ErrMat    0.00005782  MaxEl  0.00002827
<May17-2004> <14:40:53>     4  ErrMat    0.00000425  MaxEl -0.00000266
<May17-2004> <14:40:55>     5  ErrMat    0.00000055  MaxEl  0.00000026
<May17-2004> <14:40:55>  SCF converged
<May17-2004> <14:40:57>     6  ErrMat    0.00000007  MaxEl -0.00000004
<May17-2004> <14:40:57>  >>>> TOTEN
<May17-2004> <14:41:02>  >>>> POPAN
<May17-2004> <14:41:02>  >>>> DEBYE
<May17-2004> <14:41:02>  >>>> AMETS
<May17-2004> <14:41:02>  >>>> FOCKC
<May17-2004> <14:41:04>  >>>> ENGRAD
<May17-2004> <14:41:07>  ...
<May17-2004> <14:41:07>   Skipping symmetry-equivalent displacements
<May17-2004> <14:41:07>  ...
<May17-2004> <14:41:07>  Force Constants computed
<May17-2004> <14:41:07>  NORMAL TERMINATION
<May17-2004> <14:41:07>  END
<May17-2004> <14:41:08>  DENSF 2003.01  RunTime: May17-2004 14:41:08
<May17-2004> <14:41:09>  NORMAL TERMINATION
<May17-2004> <14:41:09>  END
Job /adfhome/tutorial/water IR spectrum.run has finished
```

The calculation has finished, and in the next section we will have a look at the spectrum. During the calculation of the frequencies, ADF makes a lot of small changes to the geometry of the molecule. Just for fun, you can have a look at these steps using ADFmove:

```
Select the 'Movie' command from the 'SCM' menu (in either ADFinput or ADFtail)
Rotate the image to get a better view
Press the Play button again
```



Now close the movie window.

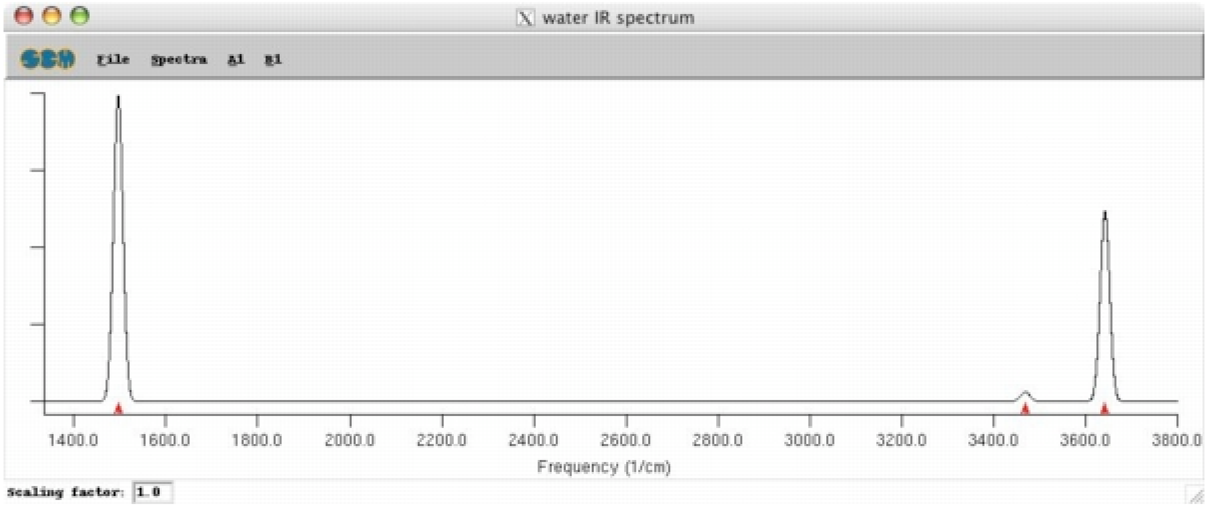
```
Select 'Quit' from the 'File' menu in ADFmovie
```

View IR spectrum

The IR spectrum has just been calculated by ADF. For detailed information you can study the textual output file of the calculation. For a graphical view, use the Spectra command from the SCM menu:

```
Select the 'Spectra' command from the 'SCM' menu
```

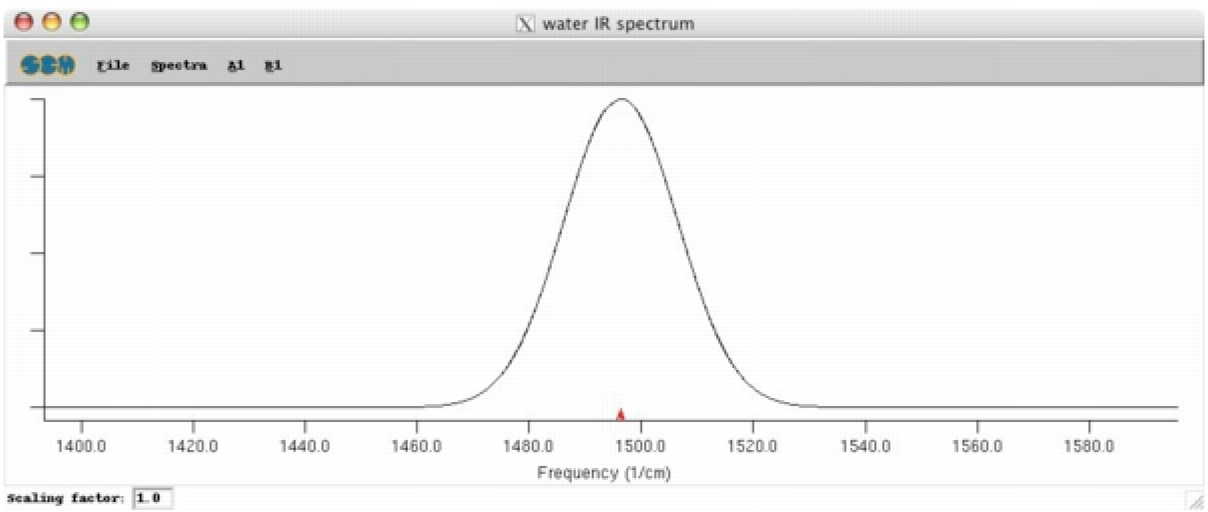
A new window will appear showing the IR spectrum of water:



The red arrows on the baseline indicate the peak positions as calculated by ADF. The peak positions, with their symmetry and intensity information, is also available from the menu.

By dragging a rectangle on a certain region in the spectrum you may zoom in:

```
Press the mouse button at the 1400 marker on the baseline of the spectrum, and hold down the mou:
Move the mouse to create a rectangle around the first peak
Release the mouse button
```



To revert to the original spectrum use the menu:

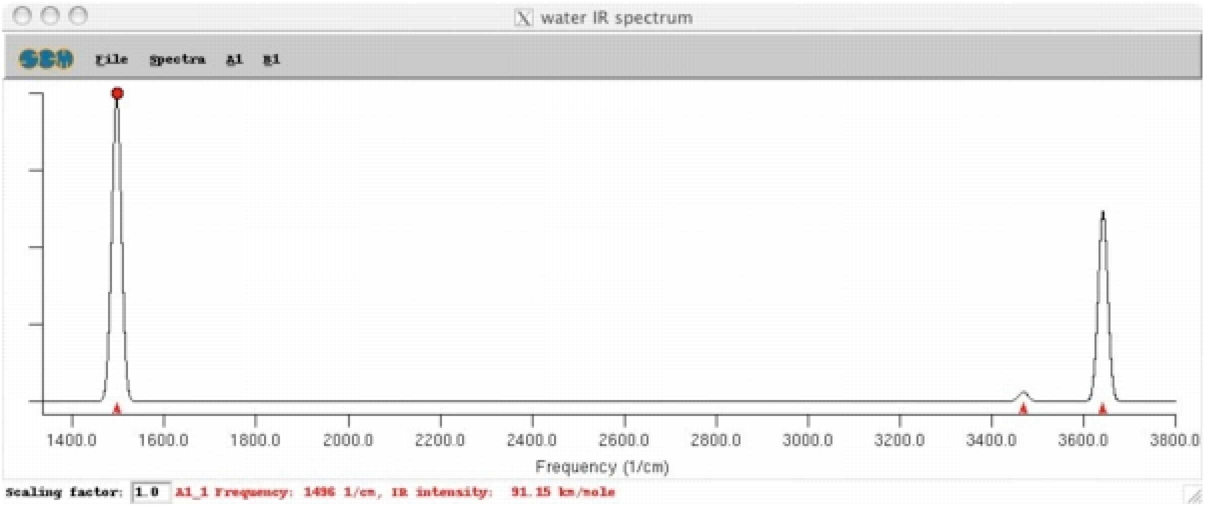
```
Select the 'Vibration' command form the 'Spectra' menu
```

If you wish to scale the frequencies you can enter a number other then 1.0 in the scale box.

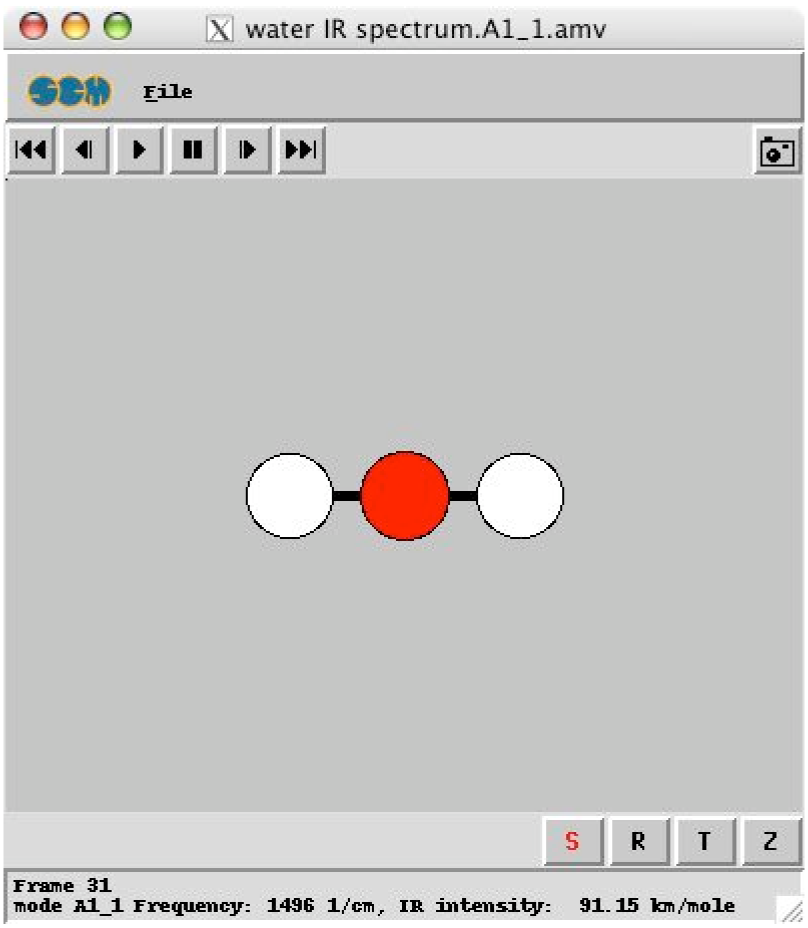
View normal modes

To get more detailed information on a peak just click on it. Below the spectrum some information will be printed, and ADFmovie will start showing the corresponding normal modes.

```
Click on the left peak
```



Note that the selected peak is marked with a dot on top of it



The atoms are moving, according to the normal mode displayed.

If you now click on a different peak, the ADFmovie windows showing the current normal modes will be closed, and new windows corresponding to the new peak will appear. By control-clicking on a peak the new windows will appear, but the old windows will not be closed.

```
Click on a different peak
Control-click on a different peak
```

If you look at the files currently in the tutorial directory you will find the following:

```
% ls
tutorial.adf                    water IR spectrum.A1_2.amv      water IR spectrum.t41
tutorial.err                    water IR spectrum.B1_1.amv      water.adf
tutorial.logfile                water IR spectrum.adf           water.err
tutorial.out                    water IR spectrum.err           water.logfile
tutorial.run                    water IR spectrum.logfile       water.out
tutorial.t13                    water IR spectrum.out           water.run
tutorial.t21                    water IR spectrum.run           water.t13
tutorial.t41                    water IR spectrum.t13           water.t21
water IR spectrum.A1_1.amv      water IR spectrum.t21           water.t41
```

The files with .amv extension are ADF movie files. Basically, they are just text files with series of coordinates, for several frames of the movie. Furthermore you see the different text and binary files that have been created during the tutorial.

You may now close all ADFGUI windows currently open, if you wish.

Part 2: excitation spectrum

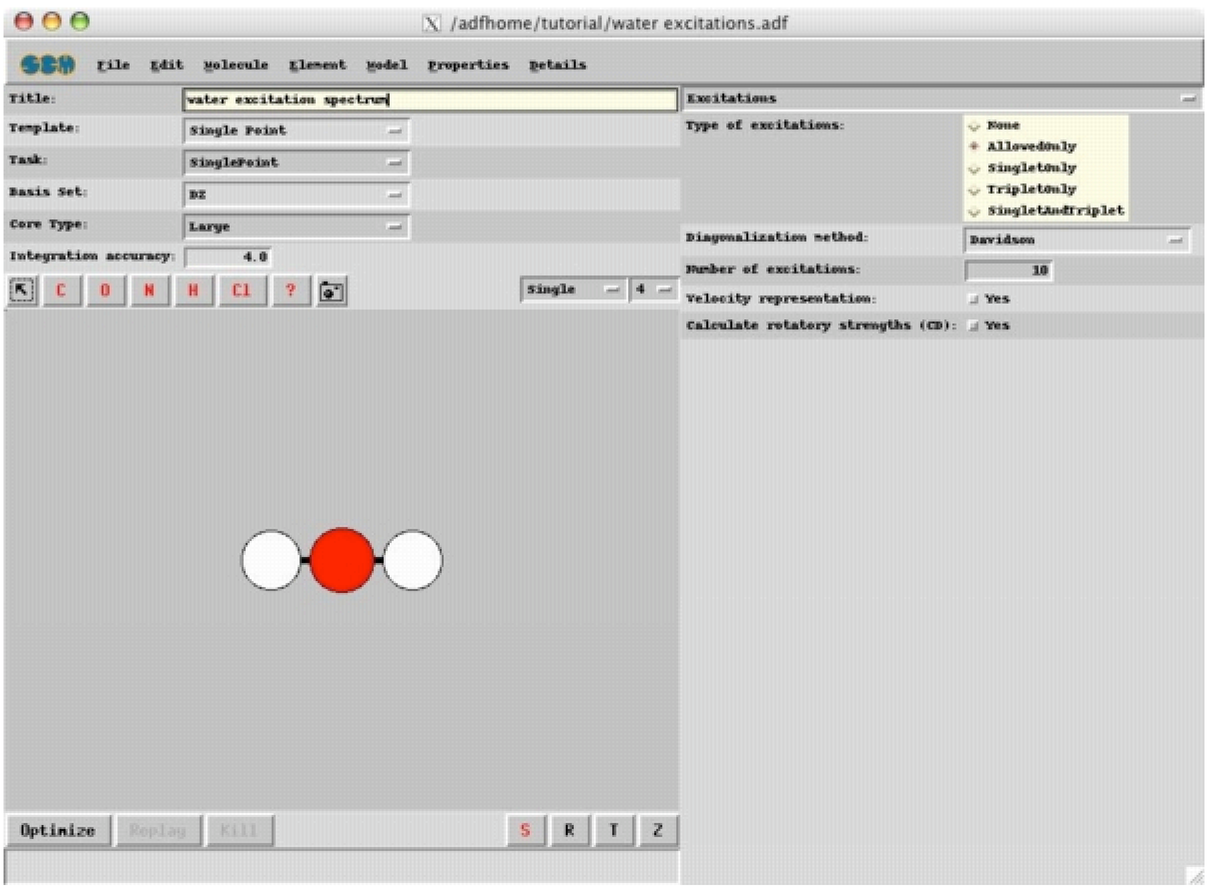
Calculate the excitation data

To show an excitation spectrum of course first we need ADF to calculate it. For this we start once again with the optimized water molecule created in this tutorial:

```
cd $ADFHOME/tutorial
adfinput water.adf &
```

Next we set up the excitation calculation:

```
Select the 'Single Point' template
Enter a proper title: 'water excitation spectrum'
Select the 'Excitations' panel (from the pull down, or from the Properties menu)
Select 'AllowedOnly'
Use the 'SaveAs...' command from the 'File' menu to save the setup as 'water excitations'
```



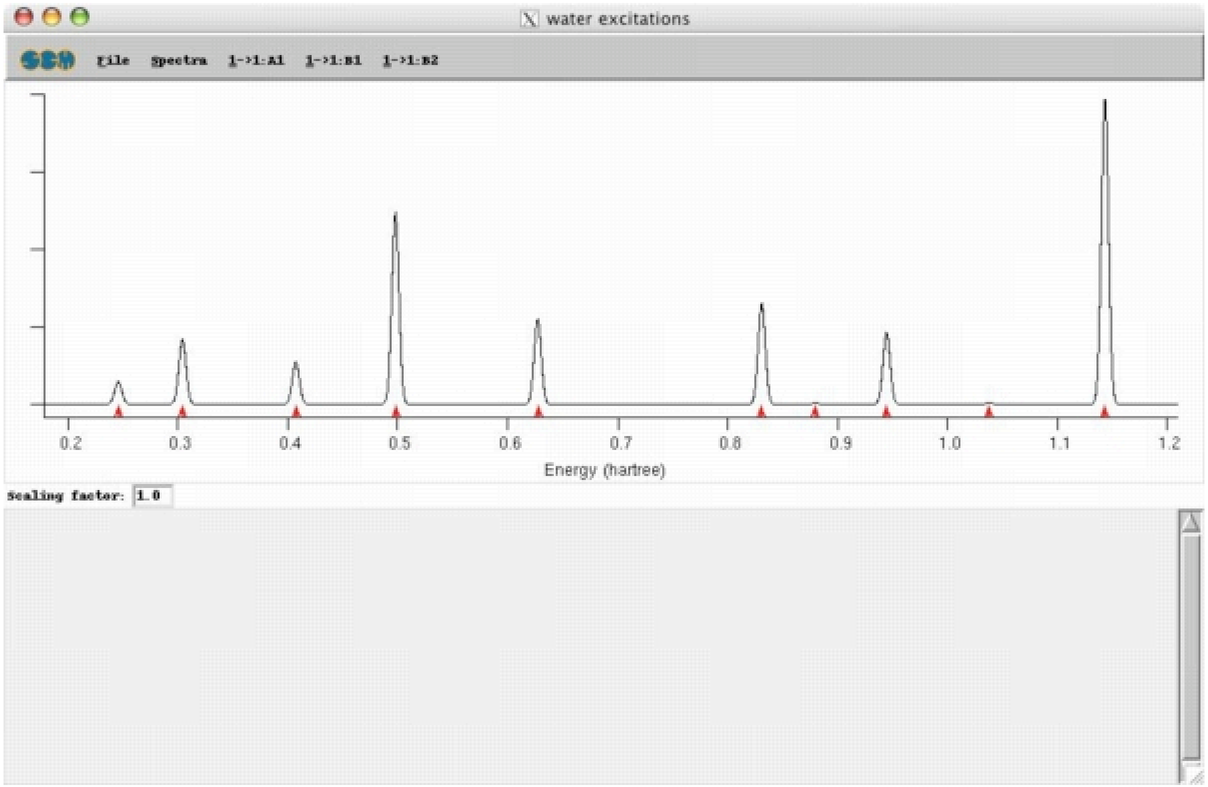
Now we are ready to run the calculation, and wait for it to finish.

```
Select the 'Run' command from the 'File' menu
Wait until the calculation is ready
```

Show the excitation spectrum

The excitation energies and intensities have been calculated, and you can find the details in the ADF textual output file. To visualize the spectrum use the ADFspectra module:

```
Select the 'Spectra' command from the 'SCM' menu
```



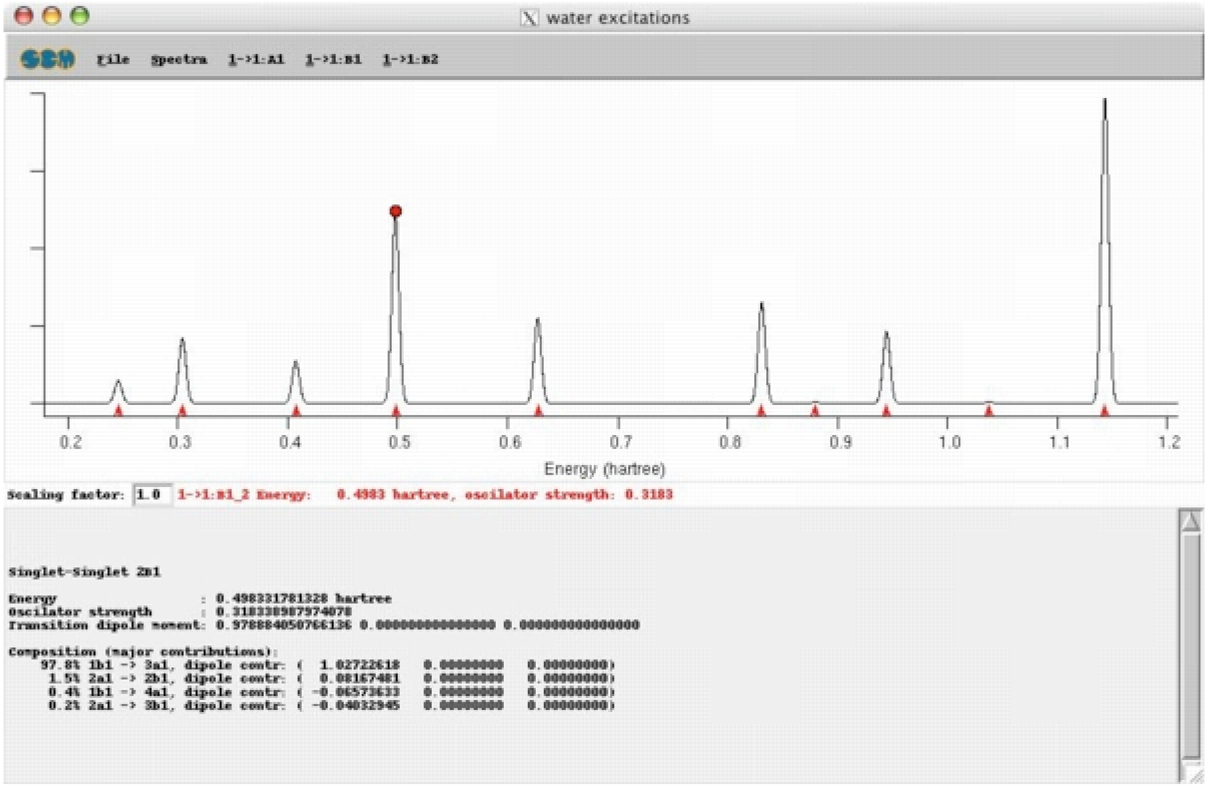
You can zoom in on parts of the spectrum by drawing a rectangle around the interesting part, just as with the IR spectrum. To get back to the full spectrum use the Spectrum menu.

```
Zoom in using the mouse
Select the 'Excitation' command from the 'Spectra' menu to revert to the full spectrum
```

Show details of excitations

The excitation energies are listed in the menus, together with details like intensity. You can select a peak using the menu or by clicking on it.

```
Click on the peak at approx. 0.5 eV
```



The peak will be selected, and detailed information about that peak, including the composition of the corresponding transition, will be printed in the lower part of the window.